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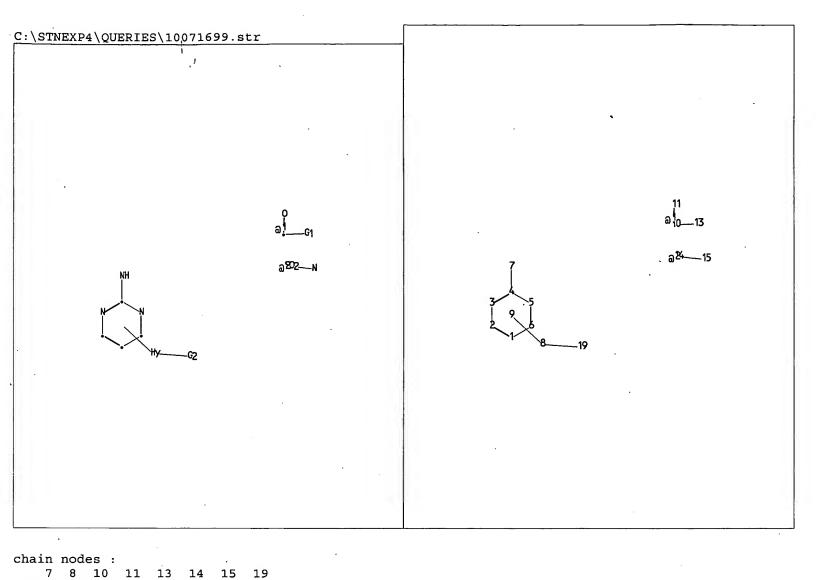
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chain bonds :
   4-7 8-19 10-11
                    10-13
ring bonds :
   1-2 1-6 2-3 3-4 4-5
exact/norm bonds :
   4-7 8-19 10-11 10-13
normalized bonds :
   1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
   containing 1 :
G1:0,N
G2:[*1],[*2]
Match level:
   1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:CLASS 10:CLASS
   11:CLASS 13:CLASS 14:CLASS 15:CLASS
                                         19:CLASS
Generic attributes :
   8:
   Saturation
                          : Unsaturated
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   Type of Ring System
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Element Count :
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14 15 19

ring nodes : 1 2 3 4

> Node 8: Limited C,C1-4

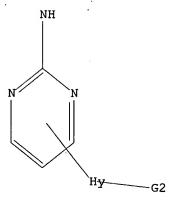
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STRUCTURE UPLOADED

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L1 HAS NO ANSWERS

L1



G1 O,N G2 [@1],[@2]

Structure attributes must be viewed using STN Express query preparation.

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1000 ITERATIONS 9.9% PROCESSED INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

1 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 196219 TO 208261

PROJECTED ANSWERS: 12 TO 392

L2 1 SEA SSS SAM L1

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SEARCH TIME: 00.00.06

237 ANSWERS

L3 237 SEA SSS FUL L1

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(FILE 'HOME' ENTERED AT 19:01:06 ON 01 JUL 2003)

FILE 'REGISTRY' ENTERED AT 19:01:10 ON 01 JUL 2003

L1 STRUCTURE UPLOADED

L2 1 S L1 SSS SAM

L3 237 S L1 SSS FUL

FILE 'CAPLUS' ENTERED AT 19:02:12 ON 01 JUL 2003

=> s 13

L4 20 L3 ·

=> d 14 1-20 bib, ab, hitstr

```
L4
     ANSWER 1 OF 20 CAPLUS COPYRIGHT 2003 ACS
AN
     2003:154244 CAPLUS
     138:187786
DN
ΤI
     Preparation of pyrimidinylthiazoles as antiinflammatories.
IN
     Love, Christopher John; Van Wauwe, Jean Pierre Frans; De Brabander, Marc
     J.; Moses, Roger Clive; Goncharenko, Mykhalyo; Cooymans, Ludwig Paul;
     Vandermaesen, Nele; Diels, Gaston Stanislas Marcella; Sibley, Anthony
     William; Noula, Caterina
PA
     Janssen Pharmaceutica N.V., Belg.
SO
     PCT Int. Appl., 97 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                       KIND
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                                              APPLICATION NO.
                                                                DATE
                              20030227
PΙ
     WO 2003015776
                                              WO 2002-EP8956
                        A1
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             TJ, TM
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              PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
             NE, SN, TD, TG
PRAI EP 2001-203088
                             20010813
     MARPAT 138:187786
OS
     Use of title compds. [I; Z = halo, alkyl; hydroxyalkyl, carboxyalkyl,
AΒ
     cyanoalkyl, aminoalkyl, aminoalkyl, aminocarbonylalkyl, alkoxyalkyl,
     polyhaloalkyl, alkoxy, cyano, amino, aminocarbonyl, aminocarbonyl,
     alkyloxycarbonyl, alkylcarbonyloxy, etc.; Q = (substituted) cycloalkyl, furyl, thienyl, pyrrolyl, oxazolyl, thiazolyl, imidazolyl, pyridyl, pyrimidinyl, pyrazinyl, pyridazinyl, benzothiazolyl, benzoxazolyl,
     benzimidazolyl, indazolyl, imidazopyridyl, etc.; L = substituted Ph,
     (substituted) monocyclic 5-6 membered partially satd. or arom.
     heterocycle, bicyclic partially satd. or arom. heterocycle] for the manuf.
     of a medicament for the prevention or the treatment of diseases mediated
     through tumor necrosis factor-alpha (TNF-.alpha.) and/or interleukin-12
     (IL-12), is claimed. Thus, Me 3-[4-methyl-2-(4-methyl-2)]
     trifluoromethylphenyl)thiazol-5-yl]-3-oxopropanoate was added to a mixt.
     prepd. from NaOMe and diguanidine carbonate in EtOCH2CH2OH followed by 3 h
     reflux to give 76% 5- (2-aminopyrimidin-4-yl)-4-methyl-2-(4-
     trifluoromethylphenyl)thiazole. The latter at 10-8 M gave 92% inhibition
     of IL-12p70.
IT
     499796-18-8P -
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (prepn. of pyrimidinylthiazoles as antiinflammatories)
RN
     499796-18-8 CAPLUS
CN
     4-Thiazolecarboxamide, 5-(2-amino-4-pyrimidinyl)-2-[4-
     (trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)
```

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4ANSWER 2 OF 20 CAPLUS COPYRIGHT 2003 ACS

AN 2002:928744 CAPLUS

DN 138:287622

TI Solid-phase synthesis of 2-(4-carbamoylpyrazolyl)-4-alkylamino-6aminopyrimidine derivatives

AU Haruta, Makoto; Ejima, Akio; Tanaka, Hiroshi; Takahashi, Takashi

CS Discovery Res. AD New Product Res. Lab., Daiichi Pharmaceutical Co. Ltd., 16-13, Kita-Kasai 1-Chome Edogawa-ku, Tokyo, Japan Heterocycles (2002), 58, 79-83 CODEN: HTCYAM: ISSN 0385-5414

SO

PB Japan Institute of Heterocyclic Chemistry

DT Journal

English LA

OS CASREACT 138:287622

AB Solid-phase synthesis of 2-(4-carbamoylpyrazolyl)-4-alkylamino-6aminopyrimidines, e.g. I, was accomplished via amination/amidation of solid supported phenol derivs. II (R = NHCH2C6H4OH-4). The methodol. allows the construction of a library of 2-(1-pyrazolyl)pyrimidines.

IT 504434-50-8P 504434-52-0P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(solid-phase synthesis of (carbamoylpyrazolyl)(alkylamino)aminopyrimidi ne derivs. via amination/amidation)

RN504434-50-8 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-[6-chloro-2-[[[4-[(2methoxyethoxy)methoxy]phenyl]methyl]amino]-4-pyrimidinyl]-5-methyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 504434-52-0 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-[6-chloro-2-[[(4hydroxyphenyl)methyl]amino]-4-pyrimidinyl]-5-methyl-, ethyl ester (9CI) (CA INDEX NAME)

IT 256930-33-3P 504434-55-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (solid-phase synthesis of (carbamoylpyrazolyl)(alkylamino)aminopyrimidi ne derivs. via amination/amidation)

RN 256930-33-3 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-(2-amino-6-chloro-4-pyrimidinyl)-5-methyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 504434-55-3 CAPLUS

CN 1H-Pyrazole-4-carboxamide, 1-[2-amino-6-(4-morpholinyl)-4-pyrimidinyl]-5-methyl-N-(2-phenylethyl)- (9CI) (CA INDEX NAME)

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

VOLUME 138

CODEN: CHABA8

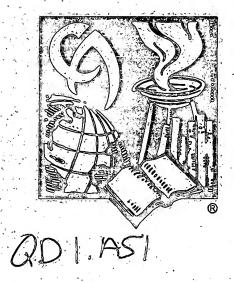
NUMBER 19

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A publication of CHEMICAL ABSTRACTS SERVICE published weekly by

A THE AMERICAN CHEMICAL SOCIETYA



RECEIVED

(PART 1 of 2 PARTS)

MAY 12, 2003

14138: 287621e "Improved cyclization process for synthesis of trimethoprim from 3,4,5" trimethoxybenzaldehyde. Wang Lin; "Yang, Hao; "Chen, "Wen-Tao; "Xing, Wen-Ru; "Yao, Xing-Zhi" (Department of Chemistry, "Nanyang Teachers College, Nanyang, "Peop "Rep." China 473061). Yingyong Huaxue 2002, 19(11), 1072–1075 (Ch), Yingyong Huaxue Bianji Weiyuanhui. Title compd. was prepd. from 3,4,5-trimethoxybenzaldehyde and β -methoxypropionitrile via condensation, forming α -(3,4,5-trimethoxybenzyl)- β -dimethoxypropionitrile, further cyclization with guanidine nitrate, got the product with yield 90%. The cyclization process was carried out by double reflux instead of conventional single reflux, and at the cyclization stage a solvent was added to the reaction mixt. The cyclization conditions were obtained by orthogonal factors and single factors expts.

138: 287622f Solid-phase synthesis of 2-(4-carbamoylpyrazolyl)-4-alkylamino-6-aminopyrimidine derivatives. Haruta, Makoto; Ejima, Akio; Tanaka, Hiroshi; Takahashi, Takashi (Discovery Res. Lab. New Product Res. Lab., Daiichi Pharmaceutical Co. Ltd., 16-13; Kita-Kasai 1-Chöme Edogawa-ku, Tokyo, Japan). Heterocycles 2002, 58, 79-83 (Eng), Japan Institute of Heterocyclic Chemistry. Solid-phase synthesis of 2-(4-carbamoylpyrazolyl)-4-alkylamino-6-

aminopyrimidines, e.g. I, was accomplished via amination/amidation of solid supported phenol derivs. II $(R = NHCH_2C_6H_4OH-4)$. The methodol. allows the construction of a library of 2-(1-pyrazolyl)pyrimidines.

138: 287623g Asymmetric synthesis of 4,6-disubstituted 1,2,3,4,5,6-hexahydro-5-hydroxypyrimidin-2-ones as potential HIV-protease-inhibitors. Enders, Dieter; Wortmann, Lars (Inst. Organische Chemie, RWTH Aachen, 52074 Aachen, Germany). Heterocycles 2002, 58, 293-299 (Eng), Japan Institute of Heterocyclic Chemistry. Hydroxy-substituted hexahydropyrimidinones I (R¹ = R² =

Me₂CH, Bu, PhCH₂, PhCH₂CH₂; $R^1 = PhCH_2CH_2$, $R^2 = PhCH_2$), potential HIV protease inhibitors, were enantioselectively prepd. in five steps starting from readily available 1,3-dibenzyl-2,5-tetrahydropyrimidinedione (II). The key step of the synthesis is the auxiliary directed stereoselective alkylation of hydrazone III, prepd. from II and (S)-1-amino-2-methoxymethylpyrrolidine (SAMP).

138: 287624h Preparation of the derivatives of 5-arylidenebabituric acid by grinding method. Geng, Li-Jun; Wang, Shu-Xiang, Li, Ji-Tai; Liu, Chun-Hong (College Chem. Environmental Sci., Hebei Univ., Boading, Peop. Rep. China 071002). Youji Huaxue 2002, 22(12), 1047-1049 (Ch), Kexue Chubanshe. Grinding a mixt. of benzaldehydes, barbituric acid and ZnCl₂ at room temp. (without any solvents) gave 5-arylidenebabituric acid in high yields, providing a simple and efficient route to these compds.

138: 287625j [1,2,4]Triazolo[1,5-c]quinazolin-2(3H)-ones and their thio analogues: a one pot synthesis. Rajan, K. Subramanian; Raghu Ram Rao, A.; Mogilaiah, K.; Prasad, M. Raghu (Medicinal Chemistry Division, University College of Pharmaceutical Sciences, Kakatiya University, Warangal, 506 009 India). Journal of Chemical Research, Synopses 2002, (10), 490-492 (Eng), Science Reviews. A facile

synthetic route for 5-aryl[1,2,4]triazolo[1,5-c]quinazolin-2(3H)-ones and 2(3H)-thiones I (X = 0, S, Ar = Ph, 4-MeC₆H₄, 2-MeOC₆H₄, 3-MeOC₆H₄, 4-MeOC₆H₄, 4-BrC₆H₄, 4-O₂NC₆H₄) has been developed. Cyclization of 3,1-benzoxazin-4(3H)-ones with semicarbazide or semithiocarbazide gave I in good yields under anhyd. conditions. This work is part of an effort to develop new bronchodilators for the treatment of asthma.

138: 287626k Attachment of Unreactive Amines to the Solid Support: Synthesis of Phenyl-Substituted Anilines, 2-Aminopyridines, and 2-Aminopyrimidines. Zhu, Shirong; Shi, Shuhao, Gerritz, Samuel W.; Sofia, Michael J. (Bristol-Myers Squibb, Wallingford, CT 06492 USA). Journal of Combinatorial Chemistry 2003, 5(3), 205-207 (Eng), American Chemical Society. An efficient method to

attach unreactive amines, e.g., anilines, aminopyridines and aminopyrimidines, to Wang resin via the carbamate linker has been developed. Increasing the reactivity of the haloarylamines by deprotonation with sodium bis(trimethylsilyl)amide was key to successfully attaching the amine to the resin. To exemplify the utility of this approach, a small library of phenyl-substituted aryl—and heteroaryl amines was synthesized via Suzuki coupling of the immobilized haloarylamine with a range of phenylboronic acids.

or pnenylooronic acids:

138: 287627m Suzuki Cross—Coupling of Solid—Supported Chloropyrimidines with Arylboronic Acids. Wade, Janice V.; Krueger, Clinton A. (ChemRx Division, Discovery Partners International Inc., South San Francisco, CA 94080 USA): Journal of Combinatorial Chemistry 2003, 5(3), 267–272 (Eng.), American Chemical Society. The util-

ity of the Suzuki cross—coupling to synthesize biaryl compds, is expanded herein to include reactions of resin—supported chloropyrimidines with boronic acids. In particular, an efficient method is described for the synthesis of a library of biaryl compds, from solid—supported chloropyrimidines. The Suzuki reaction was performed in an inert atm. using $Pd_2(dba)_3/P(t-Bu)_3$ as catalyst, spray—dried KF as base, and THF as solvent. The reaction was allowed to proceed overnight at 50 °C. Upon cleavage with acid, a library of 4—(substituted amino)—6—arylpyrimidines, e.g. I, was obtained in moderate yield and high purity.

138: 287628n Solution— and Solid—Phase Parallel Synthesis of 4—Alkoxy—Substituted Pyrimidines with High Molecular Diversity. Font, David; Heras, Montserrat; Villalgordo, Jose, M. (Departament de Quimica Facultat de Ciencies, Universitat de Girona, Girona, Spain E—17071). Journal of Combinatorial Chemistry 2003, 5(3), 311—321 (Eng), American Chemical Society. A simple and straightforward methodol. toward the synthesis of novel 2,6—disubstituted—4—alkoxypyrimidine derivs. has been developed. This methodol., initially developed in soln., can be perfectly adapted to the solid support under analogous conditions, taking full advantage of automated parallel synthesis systems. This successful methodol. benefits from the key role played by the thioether linkage placed at the 2—position in a double manner: on one side, the steric effect exerted by the thioether linkage is likely to be responsible for the very high obsd. selectivity toward the formation of the O—alkylation products. On the other side, this sulfur linkage can serve not only as a robust point of attachment for the heterocycle, stable to a no. of reaction conditions, but also as a means of introducing a new element of diversity through activation to the sulfone (safety—catch linker concept) and subsequent ipso—substitution reaction with a variety of different N—nucleophiles.

138: 287629p Studies on Quinazolines. 11.Intramolecular Imidate—Amide Rearrangement of 2—Substituted 4—(ω—Chloroalkoxy)quinazoline Derivatives. 1,3—O—N Shift of Chloroalkyl Groups via Cyclic 1,3—Azaoxonium Intermediates. Chen, Grace Shiahuy; Kalchar, Shivaramayya; Kuo, Chun—Wei; Chang, Chih—Shiang; Usifoh, Cyril O.; Chern, Ji—Wang (School of Pharmacy, College of Medicine, National Taiwan University, Taipei, Peop. Rep. China 100). Journal of Organic Chemistry 2003, 68(6), 2502—2505 (Eng), American Chemical Society. The ω—chloroalkylation of 2—substituted quinazolin—4(3H)—

one derivs. I (R = PH, Bn) with $Br-(CH_2)_n-Cl$ (n = 2-4) and the intramol imidate-amide rearrangement of the alkylated products are described. 'At room temp, the 2-Ph substituent promoted O-alkylation, whereas the less steric 2-benzyl group led to a higher ratio of

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ANSWER 3 OF 20 CAPLUS COPYRIGHT 2003 ACS
L4
AN
     2002:849620
                 CAPLUS
DN
     137:353031
ΤI
     Preparation of 4-aryltriazoles useful in treating diseases associated with
     unwanted cytokine activity
ΙN
     Tullis, Joshua Spector; Van Rens, John Charles; Clark, Michael Philip;
     Blass, Benjamin Eric; Natchus, Michael George; De, Biswanath
PA
     The Procter & Gamble Company, USA
     PCT Int. Appl., 62 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
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                                           APPLICATION NO.
                                                             DATE
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             FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG,
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     US 2003100558
                            20030529
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                       A1
                                                             20020424
PRAI US 2001-287604P
                            20010430
     MARPAT 137:353031
os
AB
     The present invention relates to 4-aryltriazoles (shown as I; e.g.
     4-(4-Fluorophenyl)-5-[2-[(phenylmethyl)amino]pyrimidin-4-yl]-1-
     ethoxymethyl-1,2,3-triazole) wherein R1 is independently: lower alkyl,
     lower alkenyl, lower alkynyl, lower heteroalkyl, lower heteroalkenyl,
     lower heteroalkynyl, heterocycloalkyl, heteroaryl, halo, CN, OR4, SR4,
     S(0)R4, S(0)2R4, and NR4R5; Q is II or III, and other variables are
     defined in the claims. Said compds. are useful in treating diseases
     assocd. with unwanted cytokine activity, inter alia, interleukin-1 (IL-1)
     and tumor necrosis factor (TNF) from cells, e.g. osteoarthritis,
     rheumatoid arthritis, and congestive heart failure (no data). Although
     the methods of prepn. are not claimed, several example prepns. are
     included and about 70 specific claimed compds. are listed.
     474557-12-5P, 4-(4-Fluorophenyl)-5-[2-((R)-1-
     phenylethylamino)pyrimidin-4-yl]-1-ethoxycarbonyl-1,2,3-triazole
     474557-14-7P 474557-15-8P, 4-(4-Fluorophenyl)-5-[2-((R)-
     1-phenylethylamino)pyrimidin-4-yl]-1-(2-methoxyethoxycarbonyl)-1,2,3-
     triazole 474557-25-0P, 4-(4-Fluorophenyl)-5-[2-((R)-1-
     phenylethylamino)pyrimidin-4-yl]-1-(N-ethyl-N-phenylaminocarbonyl)-1,2,3-
     triazole 474557-27-2P, 4-(4-\text{Fluorophenyl})-5-[2-((R)-1-
     phenylethylamino)pyrimidin-4-yl]-1-(N,N-dimethylaminocarbonyl)-1,2,3-
     triazole
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (drug candidate; prepn. of aryltriazoles useful in treating diseases
        assocd. with unwanted cytokine activity)
RN
     474557-12-5 CAPLUS
CN
     1H-1,2,3-Triazole-1-carboxylic acid, 4-(4-fluorophenyl)-5-[2-[[(1R)-1-fluorophenyl)]]
     phenylethyl]amino]-4-pyrimidinyl]-, ethyl ester (9CI) (CA INDEX NAME)
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Absolute stereochemistry.

RN 474557-14-7 CAPLUS

CN 1H-1,2,3-Triazole-1-carboxylic acid, 4-(4-fluorophenyl)-5-[2-[[(1R)-1-phenylethyl]amino]-4-pyrimidinyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 474557-15-8 CAPLUS

CN 1H-1,2,3-Triazole-1-carboxylic acid, 4-(4-fluorophenyl)-5-[2-[[(1R)-1-phenylethyl]amino]-4-pyrimidinyl]-, 2-methoxyethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 474557-25-0 CAPLUS

CN 1H-1,2,3-Triazole-1-carboxamide, N-ethyl-4-(4-fluorophenyl)-N-phenyl-5-[2-[(1R)-1-phenylethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 474557-27-2 CAPLUS

CN 1H-1,2,3-Triazole-1-carboxamide, 4-(4-fluorophenyl)-N,N-dimethyl-5-[2-[(1R)-1-phenylethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 4 OF 20 CAPLUS COPYRIGHT 2003 ACS
L4
AN
     2002:814126 CAPLUS
DN
     137:325327
     Preparation of thienyl-substituted pyrimidinyl, pyridinyl and triazinyl
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     amines as inhibitors of c-Jun N-terminal kinases (JNK) and other protein
     Cao, Jingrong; Green, Jeremy; Moon, Young-Choon; Wang, Jian; Ledeboer,
IN
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                                                         Common Juneutois
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PA
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     PCT Int. Appl., 137 pp.
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    WO 2002083667
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                                           US 2002-121035
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PRAI US 2001-283621P
                      Ρ
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    US 2001-292974P
                      Ρ
                            20010523
    US 2001-329440P
                       Ρ
                            20011015
    MARPAT 137:325327
    The present invention provides thienyl-substituted pyrimidinyl, pyridinyl
    and triazinyl amines (shown as I, e.g. 2-methylsulfanyl-5-(2-
    phenylaminopyrimidin-4-yl)-4-(4-chlorophenyl)thiophene-3-carbonitrile): or
    a pharmaceutically acceptable deriv. thereof, wherein A, B, Ra, R1, R2, R3
    and R4 are as described in the specification. These compds. are
    inhibitors of protein kinase, particularly inhibitors of JNK, a mammalian
    protein kinase involved in cell proliferation, cell death and response to
    extracellular stimuli; Lck and Src kinase. The invention also provides
    pharmaceutical compns. comprising the inhibitors of the invention and
    methods of using those compns. in the treatment and prevention of various
    disorders. Although the methods of prepn. are not claimed, 42 example
    prepns. of intermediates and I are included. Results of JNK, Src and Lck
    inhibition are tabulated for many I.
IT
     473531-16-7P, 2-((Ethylamino)carbonyl)-3-(trifluoromethyl)-4-
     (pyridin-3-yl)-5-(2-(benzylamino)pyrimidin-4-yl)thiophene
     473531-17-8P 473531-18-9P, 2-(Nitromethyl)-3-
     ((ethylamino)carbonyl)-4-((4-chlorophenyl)amino)-5-(2-aminopyrimidin-4-
    yl) thiophene 473531-32-7P, 2-(Methylamino)-3-
     ((methylamino)carbonyl)-4-phenyl-5-(2-aminopyrimidin-4-yl)thiophene
     473531-33-8P, 2-(Methylthio)-3-((methylamino)carbonyl)-4-phenyl-5-
     (2-(phenylamino)pyrimidin-4-yl)thiophene 473531-34-9P,
     2-Ethoxy-3-((methylamino)carbonyl)-4-(4-chlorophenyl)-5-(2-
     (phenylamino)pyrimidin-4-yl)thiophene 473531-71-4P,
     2-(Methylthio)-3-(ethoxycarbonyl)-4-phenyl-5-(2-((3-
    hydroxyphenyl) amino) pyrimidin-4-yl) thiophene 473531-72-5P,
```

2-(Methylthio)-3-(ethoxycarbonyl)-4-phenyl-5-(2-(phenylamino)pyrimidin-4-yl)thiophene

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; prepn. of thienyl-substituted pyrimidinyl, pyridinyl and triazinyl amines as inhibitors of JNK and other protein kinases)

RN 473531-16-7 CAPLUS

CN 2-Thiophenecarboxamide, N-ethyl-5-[2-[(phenylmethyl)amino]-4-pyrimidinyl]-4-(3-pyridinyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 473531-17-8 CAPLUS

CN 3-Thiophenecarboxamide, 2-[2-(benzoylamino)-4-pyrimidinyl]-4-(ethylamino)-N-(phenylmethyl)-5-[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ \parallel & & & \\ N & & N & \\ \parallel & & & \\ Ph-CH_2-NH-C & & NHEt \\ O & & & \\ \end{array}$$

RN 473531-18-9 CAPLUS

CN 3-Thiophenecarboxamide, 5-(2-amino-4-pyrimidinyl)-4-[(4-chlorophenyl)amino]-N-ethyl-2-(nitromethyl)- (9CI) (CA INDEX NAME)

RN 473531-32-7 CAPLUS

CN 3-Thiophenecarboxamide, 5-(2-amino-4-pyrimidinyl)-N-methyl-2-(methylamino)-4-phenyl- (9CI) (CA INDEX NAME)

RN 473531-33-8 CAPLUS

CN 3-Thiophenecarboxamide, N-methyl-2-(methylthio)-4-phenyl-5-[2-(phenylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 473531-34-9 CAPLUS

CN 3-Thiophenecarboxamide, 4-(4-chlorophenyl)-2-ethoxy-N-methyl-5-[2-(phenylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 473531-71-4 CAPLUS

CN 3-Thiophenecarboxylic acid, 5-[2-[(3-hydroxyphenyl)amino]-4-pyrimidinyl]-2-(methylthio)-4-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 473531-72-5 CAPLUS

CN 3-Thiophenecarboxylic acid, 2-(methylthio)-4-phenyl-5-[2-(phenylamino)-4-pyrimidinyl]-, ethyl ester (9CI) (CA INDEX NAME)

```
L4
     ANSWER 5 OF 20 CAPLUS COPYRIGHT 2003 ACS
ΑN
     2002:777930 CAPLUS
DN
     137:294968
TI
     Preparation of 4-(1H-pyrrolyl)pyrimidin-2-ylamines as inhibitors of cyclin
     dependent kinases for treating cancer
IN
     Fischer, Peter Martin; Wang, Shudong; Wood, Gavin
     Cyclacel Limited, UK
PA
SO
     PCT Int. Appl., 73 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                      KIND
                            DATE
                                           APPLICATION NO.
                                                             DATE
    WO 2002079193
PΙ
                       A1
                            20021010
                                           WO 2002-GB1445
                                                             20020326
             AE, AG, AL, AM, AT, AU,
                                     AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
             TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
                            (CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
             BF, BJ, CF, CG,
     GB 2375534
                            20021120
                                           GB 2002-7229
                       A1
                                                             20020327
PRAI GB 2001-7901
                            20010329
OS
    MARPAT 137:294968
AΒ
    The title compds. [I; one of \times 1 and X2 = NR10 and the other of X1 and X2 =
    CR9; Z = NH, NHCO, NHSO2, etc.; R1-R3, R9, R10 = H, alkyl, aryl, etc.;
    R4-R8 = H, alkyl, halo, etc.; with the proviso], useful as inhibitors of
     cyclin-dependent kinases (CDKs) and hence useful in the treatment of
    proliferation disorders such as cancer, leukemia, psoriasis and the like,
    were prepd. Thus, heating 3-dimethylamino-1-(2,4-dimethyl-1H-pyrrol-3-
    yl)propenone (prepn. given) with 4-fluorophenyl guanidine nitrate in the
    presence of NaOH in 2-methoxyethanol at 100-120.degree.C under N2 for 6 h
    afforded 62% II which showed IC50 of 1.0.+-.0.7 .mu.M against CDK2/cyclin
    E.
IT
     467470-28-6P
    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (drug candidate; prepn. of 4-(1H-pyrrolyl)pyrimidin-2-ylamines as
        inhibitors of cyclin dependent kinases for treating cancer)
RN
     467470-28-6 CAPLUS
CN
     1H-Pyrrole-2-carboxamide, 4-[2-[(4-fluorophenyl)amino]-4-pyrimidinyl]-3,5-
```

(CA INDEX NAME)

dimethyl- (9CI)

$$\begin{array}{c|c} O & H \\ H_2N-C & N \\ \hline Me & N \\ N & NH \\ \hline \end{array}$$

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/071,699

L4 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2003 ACS

AN 2002:767293 CAPLUS

DN 138:331295

TI Synthesis and mechanism of action of novel pyrimidinyl pyrazole derivatives possessing antiproliferative activity

AU Ohki, Hitoshi; Hirotani, Kenji; Naito, Hiroyuki; Ohsuki, Satoru; Minami, Megumi; Ejima, Akio; Koiso, Yukiko; Hashimoto, Yuichi

CS Medicinal Chemistry Research Laboratory, Paiichi Pharmaceutical Co. Ltd., Edogawa-ku, Tokyo, 134, Japan

SO Bioorganic & Medicinal Chemistry Letters (2002), 12(21), 3191-3193 CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science Ltd.

DT Journal

LA English

AB Pyrimidinyl pyrazole derivs., prepd. as a new scaffold of an anti-tumor agent, showed antiproliferative activity against human lung cancer cell lines and inhibited tubulin polymn. Furthermore, it was found that compd. I bound at the colchicine site on tubulin, but the tubulin binding pattern was different from that of colchicine. Here, we describe the synthesis of the derivs. and the differences of the action mechanism on tubulin polymn. inhibition between compd. I and colchicine.

IT 210992-71-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and tubulin polymn. inhibition of novel pyrimidinyl pyrazole derivs. possessing antiproliferative activity)

RN 210992-71-5 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-[2-[[(4-methoxyphenyl)methyl]amino]-4-pyrimidinyl]-5-methyl-, ethyl ester (9CI) (CA INDEX NAME)

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L4
     ANSWER 7 OF 20 CAPLUS COPYRIGHT 2003 ACS
AN
     2002:637673 CAPLUS
DN
     137:185518
TI
     Pyrimidine derivatives as ERK2 inhibitors
     Cao, Jingrong; Green, Jeremy; Hale, Michael; Maltais, Francois; Straub,
TN
     Judy; Tang, Qing; Aronov, Alex
Vertex Pharmaceuticals Incorporated, USA
PA
so
     PCT Int. Appl., 188 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
                                            APPLICATION NO.
     PATENT NO.
                      KIND
                            DATE
                                                              DATE
PΙ
     WO 2002064586
                            20020822
                                            WO 2002-US3791
                       A2
                                                              20020208
                            20030206
     WO 2002064586
                       A3
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
             TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     US 2003092714
                       A1 . 20030515
                                            US 2002-71699
                                                              20020208
                            20010209 <
PRAI US 2001-267818P
                       Р
                            20011012 /
     US 2001-328768P
                       P
     MARPAT 137:185518
os
     Pyrimidnes I [Z1, Z2 = N, CH; X = 5-membered heteroarom. ring to which QR2
     is attached in the 3-position relative to the pyrimidine ring attachment;
     T, Q = linker group; U = NR4, NR4CO, NR4CONR4, NR4CO2, O, CONR4, CO, CO2,
     O2C, NR4SO2, SO2NR4, NR4SO2NR4, SO2; m, n = 0, 1; R1 = CN, halogen, NR42,
     (un) substituted OH; R2 = (un) substituted alkyl, NH2; R3 = H,
     (un) substituted alkyl, CN; R4 = H, (un) substituted alkyl; NR42 =
     heterocyclic] were prepd. for use as inhibitors of ERK2 and for treating
     diseases in mammals that are alleviated by a protein kinase inhibitor,
     particularly diseases such as cancer, inflammatory disorders, restenosis,
     diabetes, and cardiovascular disease. Thus, the pyrimidine II was
     obtained by cyclizing the 3-dimethylamino-2-methylacryloylpyrrole fragment
     with (S)-HOCH2CHPhNHC(:NH)NH2. II had ki <0.1 .mu.M for inhibition of
     ERK2 in vitro.
ΙT
     449731-36-6P
     RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (prepm. of pyrimidine derivs. as ERK2 inhibitors).
RN
     449731-36-6 CAPLUS
     1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-5-methyl-4-pyrimidinyl]-N-
     [(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)
```

Absolute stereochemistry.

```
IT
     449730-24-9P 449730-37-4P 449730-39-6P
     449730-40-9P 449730-49-8P 449730-53-4P
     449730-56-7P 449730-60-3P 449730-62-5P
     449730-81-8P 449731-00-4P 449731-19-5P
     449731-20-8P 449731-21-9P 449731-22-0P
     449731-23-1P 449731-24-2P 449731-26-4P
     449731-30-0P 449731-31-1P 449731-33-3P
     449731-35-5P 449731-39-9P 449731-40-2P
     449731-41-3P 449731-43-5P 449731-44-6P
     449731-50-4P 449731-51-5P 449731-52-6P
     449731-53-7P 449731-54-8P 449731-56-0P
     449731-57-1P 449731-58-2P 449731-59-3P
     449731-60-6P 449731-62-8P 449731-63-9P
     449731-64-0P 449731-65-1P 449731-66-2P
     449731-67-3P 449731-68-4P 449731-69-5P
     449731-70-8P 449731-71-9P 449731-72-0P
     449731-73-1P 449731-74-2P 449731-75-3P
     449731-76-4P 449731-77-5P 449731-78-6P
     449731-79-7P 449731-80-0P 449731-81-1P
     449731-83-3P 449731-85-5P 449731-86-6P
     449731-87-7P 449731-88-8P 449731-89-9P
     449731-90-2P 449731-91-3P 449731-92-4P
     449731-93-5P 449731-94-6P 449731-95-7P
    449731-96-8P 449731-97-9P 449731-98-0P
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    449732-07-4P 449732-08-5P 449732-10-9P
    449732-12-1P 449732-13-2P 449732-14-3P
    449732-15-4P 449732-16-5P 449732-17-6P
     449732-18-7P 449732-19-8P 449732-20-1P
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     449732-24-5P 449732-25-6P 449732-26-7P
     449732-27-8P 449732-28-9P 449732-29-0P
    449732-30-3P 449732-31-4P 449732-32-5P
     449732-33-6P 449732-34-7P 449732-35-8P
    449732-36-9P 449732-37-0P 449732-38-1P
    449732-39-2P 449732-40-5P 449732-41-6P
    449732-42-7P 449732-43-8P 449732-44-9P
    449732-45-0P 449732-46-1P 449732-47-2P
    449732-48-3P 449732-49-4P 449732-50-7P
    449732-51-8P 449732-52-9P 449732-53-0P
    449732-54-1P 449732-55-2P 449732-56-3P
    449732-57-4P 449733-07-7P
    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
```

RN 449730-24-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-5-phenyl-4-pyrimidinyl)-N-[2-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H & O \\ N & || \\ C-NH-CH_2-CH_2 \\ \hline N & NH_2 \\ \end{array}$$

RN 449730-37-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-(3,4-dimethoxyphenyl)-4-pyrimidinyl]-N-[2-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

RN 449730-39-6 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-(3-methylphenyl)-4-pyrimidinyl]-N-[2-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 449730-40-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-(3-chlorophenyl)-4-pyrimidinyl]-N-[2-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & &$$

RN 449730-49-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-5-phenyl-4-pyrimidinyl)-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 449730-53-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-(3,4-dimethoxyphenyl)-4-pyrimidinyl]-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 449730-56-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-(3-methylphenyl)-4-pyrimidinyl]-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 449730-60-3 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-(3-chlorophenyl)-4-pyrimidinyl]-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} & \text{H} \\ & \parallel & \parallel & \text{H} \\ \text{Ph-CH}_2 - \text{N-C} & & \text{N} \\ \end{array}$$

RN 449730-62-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-(3-chloro-2-fluorophenyl)-4-pyrimidinyl]-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 449730-81-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-(3-chloro-2-fluorophenyl)-4-pyrimidinyl]-N-[(1R,2R)-2-hydroxy-1-methyl-2-phenylethyl]-N-methyl-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 449731-00-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-5-methyl-4-pyrimidinyl)-N-[[(2S)-tetrahydro-2-furanyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-19-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-(3,5-dichlorophenyl)-4-pyrimidinyl]-N-(1,3-benzodioxol-5-ylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 449731-20-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-(3,5-dichlorophenyl)-4-pyrimidinyl]-N-[2-(dimethylamino)-2-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

RN 449731-21-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-(3,5-dichlorophenyl)-4-pyrimidinyl]-N-[[4-(methylsulfonyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

Me-S

O

$$CH_2-NH-C$$
 H_2N
 N
 $C1$

RN 449731-22-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-(1,3-benzodioxol-5-ylmethyl)-4-[5-(3,5-dichlorophenyl)-2-(phenylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 449731-23-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[5-(3,5-dichlorophenyl)-2-(phenylamino)-4-pyrimidinyl]-N-[2-(4-morpholinyl)-2-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RN 449731-24-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-[3-fluoro-5-(trifluoromethyl)phenyl]-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-26-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-5-methyl-4-pyrimidinyl)-N-[2-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H & O \\ N & || \\ C-NH-CH_2-CH_2 \\ \hline N & NH_2 \\ \end{array}$$

RN 449731-30-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[5-methyl-2-(phenylamino)-4-pyrimidinyl]-N-propyl- (9CI) (CA INDEX NAME)

RN 449731-31-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[5-methyl-2-(phenylamino)-4-pyrimidinyl]-N-(3-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 449731-33-3 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-cyclopropyl-4-[2-(ethylamino)-5-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449731-35-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-(phenylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-39-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-(2-aminoethyl)-4-[5-methyl-2-(phenylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449731-40-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-4-pyrimidinyl)-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 449731-41-3 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-4-pyrimidinyl)-N-[(1R,2R)-2-hydroxy-1-methyl-2-phenylethyl]-N-methyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 449731-43-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-5-methyl-4-pyrimidinyl]-N-(3-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 449731-44-6 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-5-ethyl-4-pyrimidinyl)-N-[2-(6-methoxy-1H-indol-3-yl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & \overset{H}{\text{N}} & \overset{O}{\text{CH}_2} - \text{CH}_2 - \text{NH} - \overset{O}{\text{C}} & \overset{H}{\text{N}} & \overset{N}{\text{NH}_2} \\ & & \text{Et} & \overset{N}{\text{NH}_2} & \overset{N}{\text{$$

RN 449731-50-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[[2-(diethylamino)ethyl]amino]-5-methyl-4-pyrimidinyl]-N-[(3,4-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & &$$

RN 449731-51-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[5-methyl-2-[[2-(1-piperidinyl)-4-quinazolinyl]amino]-4-pyrimidinyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

*** FRAGMENT DIAGRAM IS INCOMPLETE ***

RN 449731-52-6 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[1-(3-chloro-4-fluorophenyl)-2-hydroxyethyl]-4-[5-methyl-2-(methylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449731-53-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[1-(3-chloro-4-fluorophenyl)-2-hydroxyethyl]-4- [5-methyl-2-(phenylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449731-54-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[(3-fluorophenyl)amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-56-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[(3-hydroxyphenyl)amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-57-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(1,3-benzodioxol-5-ylamino)-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HO S
$$\stackrel{H}{\sim}$$
 $\stackrel{N}{\sim}$ $\stackrel{N}{\sim}$

RN 449731-58-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[[4-(aminosulfonyl)phenyl]amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-59-3 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-[3-(phenylmethoxy)phenyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-60-6 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[(trans-4-hydroxycyclohexyl)amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-62-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[5-cyclopropyl-2-(phenylamino)-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-63-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[1-(3-fluoro-4-methylphenyl)-2-hydroxyethyl]-4-[5-methyl-2-(phenylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449731-64-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[2-hydroxy-1-[3-(trifluoromethyl)phenyl]ethyl]-4-[5-methyl-2-(phenylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449731-65-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[1-(3-fluoro-4-methylphenyl)-2-hydroxyethyl]-4-[2-[(3-fluorophenyl)amino]-5-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449731-66-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[(3-fluorophenyl)amino]-5-methyl-4-pyrimidinyl]-N-[2-hydroxy-1-[3-(trifluoromethyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

RN 449731-67-3 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-[[3-(trifluoromethyl)phenyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449731-68-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-[(phenylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-69-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[(3,4-dimethylphenyl)amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

RN 449731-70-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-[[4-(phenylmethoxy)phenyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-71-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-[(1-methylethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449731-72-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-[(2,2,2-trifluoroethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-73-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[2-[[(1S)-2-hydroxy-1-phenylethyl]amino]-5-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-74-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[2-[(2-methoxyphenyl)amino]-5-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449731-75-3 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-[4-(trifluoromethoxy)phenyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-76-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-[(2-methylpropyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449731-77-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[(cyclopropylmethyl)amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-78-6 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-(methoxymethyl)-2-(phenylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-79-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-(methoxymethyl)-4-pyrimidinyl]-N[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

RN 449731-80-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(cyclopropylamino)-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-81-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-(propylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-83-3 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[2-[[(1R)-2-hydroxy-1-phenylethyl]amino]-5-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449731-85-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-5-methyl-4-pyrimidinyl]-N[(1R,2S)-2-hydroxy-1-methyl-2-phenylethyl]-, rel- (9CI) (CA INDEX NAME)

Relative · stereochemistry.

RN 449731-86-6 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-5-methyl-4-pyrimidinyl]-N-(2-hydroxy-2-phenylethyl)- (9CI) (CA INDEX NAME)

RN 449731-87-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-5-methyl-4-pyrimidinyl]-N[(1S,2S)-2-hydroxy-1-(hydroxymethyl)-2-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-88-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-5-methyl-4-pyrimidinyl]-N[(1R,2R)-2-hydroxy-1-(hydroxymethyl)-2-phenylethyl]- (9CI) (CA INDEX NAME)

RN 449731-89-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-5-methyl-4-pyrimidinyl]-N-[(1R)-3-hydroxy-1-phenylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-90-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-5-methyl-4-pyrimidinyl]-N-[(1S)-3-hydroxy-1-phenylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-91-3 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[[1-(hydroxymethyl)cyclopropyl]amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI). (CA INDEX NAME)

RN 449731-92-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[(2-hydroxyethyl)amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-93-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[[(1R)-2-hydroxy-1-methylethyl]amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-94-6 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[2-[[(2R)-2-hydroxypropyl]amino]-5-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449731-95-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[2-[[(2S)-2-hydroxypropyl]amino]-5-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-96-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[(2-hydroxycyclohexyl)amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-97-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-4-pyrimidinyl)-N-[(1R,2S)-2-hydroxy-1-methyl-2-phenylethyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 449731-98-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-4-pyrimidinyl)-N-[(1R)-2-hydroxy-1-methyl-2-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-01-8 CAPLUS

CN Benzeneacetic acid, .alpha.-[[[4-[2-(ethylamino)-5-methyl-4-pyrimidinyl]-1H-pyrrol-2-yl]carbonyl]amino]-, methyl ester, (.alpha.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-05-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-5-methyl-4-pyrimidinyl]-N-[2-hydroxy-1-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

RN 449732-06-3 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-5-(hydroxymethyl)-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-07-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-5-methyl-4-pyrimidinyl]-N-[1-[3-fluoro-5-(trifluoromethyl)phenyl]-2-hydroxyethyl]- (9CI) (CA INDEX NAME)

RN 449732-08-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-5-methyl-4-pyrimidinyl]-N-[1-(3-fluorophenyl)-2-hydroxyethyl]- (9CI) (CA INDEX NAME)

RN 449732-10-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-5-methyl-4-pyrimidinyl]-N-[1-(2-fluorophenyl)-2-hydroxyethyl]- (9CI) (CA INDEX NAME)

RN 449732-12-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[[2-cyclopropyl-1-(hydroxymethyl)ethyl]amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-13-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[(2,3-dimethylphenyl)amino]-5-methyl-4-

pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-14-3 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethoxyamino)-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-15-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[[(1S)-1-(hydroxymethyl)-2-methylpropyl]amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

RN 449732-16-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-5-methyl-4-pyrimidinyl]-N-(2-oxo-1-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 449732-17-6 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-5-methyl-4-pyrimidinyl]-N[(1S)-2-hydroxy-1-[3-(trifluoromethyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-18-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[(3-fluorophenyl)amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-[3-(trifluoromethyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-19-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[(2-chlorophenyl)amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-[3-(trifluoromethyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-20-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[[(1S)-2-hydroxy-1-phenylethyl]amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-[3-(trifluoromethyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

RN 449732-21-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(cyclopropylamino)-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-[3-(trifluoromethyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-22-3 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(cyclopropylamino)-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-(2-methoxyphenyl)ethyl]- (9CI) (CA INDEX NAME)

RN 449732-23-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-1-(3-chlorophenyl)-2-hydroxyethyl]-4-[2-(cyclopropylamino)-5-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-24-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(cyclopropylamino)-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-(3-methylphenyl)ethyl]- (9CI) (CA INDEX NAME)

RN 449732-25-6 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[2-(methoxyamino)-5-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-26-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-[(1-methylethoxy)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-27-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[[3-(dimethylamino)phenyl]amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-(3-methylphenyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-28-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-(3-methylphenyl)ethyl]-4-[2-[(2-hydroxyphenyl)amino]-5-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-29-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-(3-methylphenyl)ethyl]-4-[2-[[[(1S)-2-hydroxy-1-phenylethyl]amino]carbonyl]amino]-5-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449732-30-3 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[(2,3-dimethylphenyl)amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-(3-methylphenyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-31-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[(3-fluorophenyl)amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-(3-methylphenyl)ethyl]- (9CI) (CA INDEX NAME)

RN 449732-32-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(acetylamino)-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-33-6 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-[(2-methylphenyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449732-34-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-(3-pyridinylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-35-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-[[(2S)-tetrahydro-2-furanyl]methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-36-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-[[(2R)-tetrahydro-2-furanyl]methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449732-37-0 CAPLUS

CN Hydrazinecarboxylic acid, 2-[4-[5-[[[(1S)-2-hydroxy-1-phenylethyl]amino]carbonyl]-1H-pyrrol-3-yl]-5-methyl-2-pyrimidinyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-38-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-[(3-pyridinylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449732-39-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[(cyclopropylmethoxy)amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-40-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[2-(3-isoxazolylamino)-5-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

*** FRAGMENT DIAGRAM IS INCOMPLETE ***

RN 449732-41-6 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[[(1S)-2-hydroxy-1-methylethyl]amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-(3-methylphenyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-42-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-(3-methylphenyl)ethyl]-4-[5-methyl-2-[(2-methylphenyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449732-43-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-1-(3-chlorophenyl)-2-hydroxyethyl]-4-[5-methyl-2-[(2-methylphenyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-44-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[(2-hydroxyethoxy)amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

RN 449732-45-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(2,2-dimethylhydrazino)-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-46-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-[2-(trifluoromethyl)phenyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-47-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-(4-morpholinylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-48-3 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-[(5-methyl-3-isoxazolyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

*** FRAGMENT DIAGRAM IS INCOMPLETE ***

RN 449732-49-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[[(1S)-1-(3-chloro-4-fluorophenyl)-2-hydroxyethyl]amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

RN 449732-50-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-1-(3-fluorophenyl)-2-hydroxyethyl]-4-[5-methyl-2-(phenylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-51-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-1-(3-chlorophenyl)-2-hydroxyethyl]-4-[2-[[(1S)-1-(hydroxymethyl)propyl]amino]-5-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449732-52-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-1-(3-chlorophenyl)-2-hydroxyethyl]-4-[2-[[2-hydroxy-1-(hydroxymethyl)ethyl]amino]-5-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-53-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-(3-methylphenyl)ethyl]-4-[2-[[(1S)-1-(hydroxymethyl)propyl]amino]-5-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449732-54-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-[[2-hydroxy-1-(hydroxymethyl)ethyl]amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-55-2 CAPLUS

CN lH-Pyrrole-2-carboxamide, 4-[2-[[(1S)-1-(hydroxymethyl)propyl]amino]-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

RN 449732-56-3 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[5-methyl-2-[(2-methylcyclopropyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-57-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(cyanoamino)-5-methyl-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449733-07-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-(3-chlorophenyl)-4-pyrimidinyl]-N-methyl-N-[2-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

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IT
     338403-73-9P 449730-92-1P 449730-93-2P
     449730-94-3P 449730-95-4P 449730-96-5P
     449730-97-6P 449730-98-7P 449730-99-8P
     449731-01-5P 449731-02-6P 449731-03-7P
     449731-04-8P 449731-05-9P 449731-06-0P
     449731-07-1P 449731-08-2P 449731-09-3P
     449731-10-6P 449731-11-7P 449731-12-8P
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     449731-37-7P 449731-38-8P 449731-45-7P
     449731-46-8P 449731-47-9P 449731-48-0P
     449731-49-1P 449731-55-9P 449731-61-7P
     449731-82-2P 449731-84-4P 449731-99-1P
     449732-00-7P 449732-02-9P 449732-03-0P
     449732-04-1P
    RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological.
     study); PREP (Preparation); USES (Uses)
        (prepn. of pyrimidine derivs. as ERK2 inhibitors)
RN
     338403-73-9 CAPLUS
CN
     1H-Pyrrole-2-carboxamide, 4-(2-amino-5-phenyl-4-pyrimidinyl)-N,N-dimethyl-
     (9CI) (CA INDEX NAME)
```

RN 449730-92-1 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-5-methyl-4-pyrimidinyl)-N(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 449730-93-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-5-methyl-4-pyrimidinyl)-N-[(3,4-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H & O \\ N & C-NH-CH_2 \end{array}$$

RN 449730-94-3 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-5-methyl-4-pyrimidinyl)-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449730-95-4 CAPLUS

CN 1H-Pyrrole-2-carioxamide, 4-(2-amino-5-methyl-4-pyrimidinyl)-N-[(4-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H & O \\ N & C - NH - CH_2 \end{array}$$

$$\begin{array}{c|c} H & O \\ Me & C - NH - CH_2 \end{array}$$

RN 449730-96-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-5-methyl-4-pyrimidinyl)-N-[(3-chlorophenyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H & O \\ N & \parallel \\ C-NH-CH_2 \end{array}$$

RN 449730-97-6 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-5-methyl-4-pyrimidinyl)-N-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H & O \\ N & C - NH - CH_2 \end{array}$$

$$\begin{array}{c|c} Me \\ Me \end{array}$$

RN 449730-98-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-5-methyl-4-pyrimidinyl)-N-[(3-chloro-4-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)

RN 449730-99-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-5-methyl-4-pyrimidinyl)-N-[[(2R)-tetrahydro-2-furanyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-01-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-5-methyl-4-pyrimidinyl)-N-[(1R)-3-hydroxy-1-phenylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-02-6 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-5-methyl-4-pyrimidinyl)-N-[(1S)-3-hydroxy-1-phenylpropyl]- (9CI) (CA INDEX NAME)

RN 449731-03-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(3-chloro-4-fluorophenyl)methyl]-4-(2,5-diamino-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

RN 449731-04-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-(methylamino)-4-pyrimidinyl]-N-[(3-chloro-4-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H & O \\ N & C-NH-CH_2 \end{array}$$

$$\begin{array}{c|c} C1 & F \\ N & NHMe \end{array}$$

RN 449731-05-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[5-(acetylamino)-2-amino-4-pyrimidinyl]-N-[(3-chloro-4-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)

RN 449731-06-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-[[(methylamino)carbonyl]amino]-4-pyrimidinyl]-N-[(3-chloro-4-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)

RN 449731-07-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-5-hydroxy-4-pyrimidinyl)-N-[(3-chloro-4-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & \\ & & \\ & \\ & & \\ &$$

RN 449731-08-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-[(methylamino)methyl]-4-pyrimidinyl]-N-[(3-chloro-4-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & \\ & & \\ & & \\ & \\ & & \\ & \\ & \\ & & \\ &$$

RN 449731-09-3 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-(hydroxymethyl)-4-pyrimidinyl]-N[(3-chloro-4-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & C1 \\ & & & \\ &$$

RN 449731-10-6 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(3-chloro-4-fluorophenyl)methyl]-4-[2-(cyclohexylamino)-5-[[(methylamino)carbonyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449731-11-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(acetylamino)-5-[[(methylamino)carbonyl]amino]-4-pyrimidinyl]-N-[(3-chloro-4-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)

RN 449731-12-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(3-chloro-4-fluorophenyl)methyl]-4-[5-hydroxy-2-[(methylsulfonyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449731-13-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-(methylsulfonyl)-4-pyrimidinyl]-N[(3-chloro-4-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)

RN 449731-14-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-(hydroxymethyl)-4-pyrimidinyl]-N[(3,4-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & &$$

RN 449731-15-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(cyclohexylamino)-5-methyl-4-pyrimidinyl]-N[(3,4-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)

RN 449731-16-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-(3,5-dichlorophenyl)-4-pyrimidinyl]-N-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

$$CH_2-NH-C$$

$$H_2N$$

$$N$$

$$C1$$

$$C1$$

RN 449731-17-3 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[5-(3,5-dichlorophenyl)-2-(phenylamino)-4-pyrimidinyl]-N-[[3-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

$$CH_2-NH-C$$
 N
 $C1$
 $PhNH$
 N
 $C1$

RN 449731-18-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-amino-5-(3,5-dichlorophenyl)-4-pyrimidinyl]-N-[(1R)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-25-3 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-5-propyl-4-pyrimidinyl)-N-[2-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
H & O \\
N & \parallel \\
C-NH-CH_2-CH_2
\end{array}$$

$$\begin{array}{c|c}
N \\
N \\
NH_2
\end{array}$$

RN 449731-27-5 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[5-methyl-2-(methylamino)-4-pyrimidinyl]-N-[2-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

RN 449731-28-6 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(methylamino)-4-pyrimidinyl]-N-[2-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
H & O \\
N & || \\
C - NH - CH_2 - CH_2 \\
\hline
N & NHMe
\end{array}$$

RN 449731-29-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[2-(dimethylamino)ethyl]-4-[2-(ethylamino)-5-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 449731-32-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-5-methyl-4-pyrimidinyl]-N-(1-naphthalenylmethyl)- (9CI) (CA INDEX NAME)

RN 449731-34-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-4-pyrimidinyl]-N-[[2-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 449731-37-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-4-pyrimidinyl]-N-(4-methylcyclohexyl)- (9CI) (CA INDEX NAME)

RN 449731-38-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[5-ethyl-2-(phenylamino)-4-pyrimidinyl]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 449731-45-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[5-methyl-2-(phenylamino)-4-pyrimidinyl]-N-(2-phenoxyethyl)- (9CI) (CA INDEX NAME)

RN 449731-46-8 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[5-methyl-2-(phenylamino)-4-pyrimidinyl]-N-(1-methyl-3-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 449731-47-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-(1H-benzimidazol-2-ylmethyl)-4-[5-methyl-2-(methylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & CH_2-NH-C & H \\ NH & N \\ Me & N \\ N & NHMe \\ \end{array}$$

RN 449731-48-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-1-(hydroxymethyl)-3-methylbutyl]-4-[5-methyl-2-(methylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-49-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-(1H-imidazol-4-ylmethyl)ethyl]-4-[5-methyl-2-(methylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-55-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[(1S)-2-hydroxy-1-phenylethyl]-4-[2-[(3-methoxyphenyl)amino]-5-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-61-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[5-cyclohexyl-2-(phenylamino)-4-pyrimidinyl]-N[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-82-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[5-(hydroxymethyl)-2-(phenylamino)-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-84-4 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-5-methyl-4-pyrimidinyl]-N[(1S,2R)-2-hydroxy-1-methyl-2-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449731-99-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-4-pyrimidinyl)-N-(2-hydroxy-2-phenylethyl)-N-methyl- (9CI) (CA INDEX NAME)

RN 449732-00-7 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-4-pyrimidinyl)-N-[(2S)-2-hydroxy-2-phenylethyl]-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-02-9 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-4-pyrimidinyl)-N-[(1S,2R)-2-hydroxy-1-methyl-2-phenylethyl]-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 449732-03-0 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-(2-amino-4-pyrimidinyl)-N-[(1R,2S)-2-hydroxy-1-methyl-2-phenylethyl]-N-methyl- (9CI) (CA INDEX NAME)

RN 449732-04-1 CAPLUS

CN 1H-Pyrrole-2-carboxamide, 4-[2-(ethylamino)-5-(methoxymethyl)-4-pyrimidinyl]-N-[(1S)-2-hydroxy-1-phenylethyl]- (9CI) (CA INDEX NAME)

- : L4 ANSWER 8 OF 20 CAPLUS COPYRIGHT 2003 ACS
 - AN 2002:348207 CAPLUS
 - DN 137:72550
 - TI Accelerating the Drug Optimization Process: Identification, Structure Elucidation, and Quantification of in Vivo Metabolites Using Stable Isotopes with LC/MSn and the Chemiluminescent Nitrogen Detector
 - AU Taylor, Eric W.; Jia, Weiping; Bush, Mark; Dollinger, Gavin D.
 - CS Small Molecule Drug Discovery, Chiron Corporation, Emeryville, CA, 94608, USA
 - SO Analytical Chemistry (2002), 74(13), 3232-3238 CODEN: ANCHAM; ISSN: 0003-2700
 - PB American Chemical Society
 - DT Journal
 - LA English
 - AB Most preclin. leads exhibit poor ADME/PK (absorption, distribution, excretion and plasma half-life) properties and require optimizing to increase the likelihood of becoming successful pharmaceuticals. As a means of accelerating the evaluation of these leads in vivo, the authors assessed the use of LC/MS with the chemiluminescent-nitrogen detector (CLND) and a stable isotope to identify and quantify in vivo metabolites and to measure excretion. A 14C-labeled preclin. lead that also contained two chlorine atoms was administered orally to rats, and samples of bile, urine, and plasma were collected and analyzed by LC with radiodetection and by LC/MS-CLND with the chlorine atoms used as tracers. Both methods identified seven metabolites in bile and two metabolites in urine. amt. and abundance of each metabolite was measured, and the results were equiv. for the two methods. Material balance was measured by liq. scintillation counting of the starting samples, by LC/radiodetection, and by LC/MS-CLND. All three methods yielded the same results and showed that the primary route of clearance was metab. followed by immediate excretion. This study demonstrates that LC/MS-CLND with a stable isotope is a method that can efficiently track and accurately quantify metabolites, making it possible to rapidly study ADME/PK in vivo without radiolabeling.
 - IT 440127-81-1

RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)

(accelerating drug optimization process by identification and structure elucidation and quantification of in vivo metabolites using stable isotopes with LC/MSn and chemiluminescent nitrogen detector applied to CHIR 99021)

- RN 440127-81-1 CAPLUS
- CN 1H-Imidazole-4-carboxylic acid, 2-[2-[[2-[(5-cyano-2-pyridinyl)amino]-4-(2,4-dichlorophenyl)-5-pyrimidinyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

CO₂H

PAGE 2-A

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4
    ANSWER 9 OF 20 CAPLUS COPYRIGHT 2003 ACS
ΑN
     2001:635876 CAPLUS
DN
     135:211049
TI
     Preparation of pyrimidinamines and pyridinamines as adenosine receptor
    modulators for treatment of CNS disorders
IN
     Borroni, Edilio Maurizio; Huber-Trottmann, Gerda; Kilpatrick, Gavin John;
     Norcross, Roger David
PA
     F. Hoffmann La Roche A.-G., Switz.
     PCT Int. Appl., 256 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                      KIND
                            DATE
                                           APPLICATION NO.
                                                             DATE
PΙ
                            20010830
                                           WO 2001-EP1679
    WO 2001062233
                       A2
                                                             20010215
                       А3
                            20020103
    WO 2001062233
            AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ,
             DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS,
             JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG,
             MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL,
             TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ,
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             BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                           EP 2001-927670
    EP 1261327
                       A2
                            20021204
                                                             20010215
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
    BR 2001008611
                            20030506
                                           BR 2001-8611
                                                             20010215
                       Α
    US 2001027196
                                           US 2001-788956
                            20011004.
                                                             20010220
                       A1
    NO 2002004006
                            20020822
                                           NO 2002-4006
                       Α
                                                             20020822
PRAI EP 2000-103432
                       Α
                            20000225
    WO 2001-EP1679
                       W
                            20010215
os
    MARPAT 135:211049
AΒ
    The title compds. (I) [wherein A = a bond, S, N(R), (CH2)2, CH:CH,
    C.tplbond.C, or O; X and Y = independently N:, :N, :CH, C(CN):, :C(CN),
     C(CSNH2):, or :C(CSNH2), wherein at least 1 of X or Y is N; R1 = H,
     (cyclo)alkyl, alkenyl, alkynyl, halo, CN, (alkyl)carboxylates,
     (alkyl) carbamates, alkoxy(alkyl), phenoxy(alkyl), phenylamino(alkyl),
     (un) substituted phenyl(alkyl) or amino(alkyl), morpholinyl(alkyl),
    piperidinyl(alkyl), pyridinyl(alkyl), piperazinyl(alkyl), etc.; R2 = H,
    halo, CN, NO2, acyl, carboxylate, (un) substituted alkyl, alkenyl, alkynyl,
    or Ph; R3 = alkyl or thienyl, (dihydro) furanyl, benzodioxolyl, isoxazolyl,
    pyridinyl, dihydropyranyl, pyrazinyl, aryl(alkyl)oxy, pyrazolyl,
     (un) substituted Ph, etc.; R4 and R5 = independently H, benzoyl, or
     (un) substituted phenacyl; or A and R2 taken together the with the C atoms
     to which they are attached may form a substituted thienyl group] were
    prepd. as adenosine receptor modulators. For example, treating
     3,4,5-trimethoxybenzoylacetonitrile with to NaH in DMSO, followed by addn.
     of CS2 and MeI, gave the bis(methylthio) intermediate. Cycloaddn. with
     guanidine nitrate in the presence of TEA in DMF afforded the
    pyrimidinenitrile (II), which exhibited high selectivity toward the A1 and
    A3 adenosine receptors compared to the A2 receptor with pKi values of
     5.88, 5.71 and 7.24, resp. I are useful for the treatment of Alzheimer's
    disease, Parkinson's disease, neuroprotection, schizophrenia, anxiety,
    pain, respiration deficits, depression, asthma, allergic responses,
    hypoxia, ischemia, seizure, substance abuse, and sedation, and they may be
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active as muscle relaxants, antipsychotics, antiepileptics, anticonvulsants, and cardioprotective agents (no data). The most preferred indications for I are those which include disorders of the central nervous system, such as certain depressive disorders, neuroprotection, and Parkinson's disease.

IT 357288-99-4P

CN

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of pyrimidinamines and pyridinamines as adenosine receptor modulators for treatment of CNS disorders and other diseases)

RN 357288-99-4 CAPLUS

2-Furancarboxylic acid, 5-[2-amino-5-cyano-6-(methylthio)-4-pyrimidinyl]-, ethyl ester (9CI) (CA INDEX NAME)

```
L4
     ANSWER 10 OF 20 CAPLUS COPYRIGHT 2003 ACS
AN
     2001:10085 CAPLUS
     134:86238
DN
TI
     Preparation of pyrazole derivatives as antitumor agents
                                                                        Con note
     Ejima, Akio; Ohsuki, Satoru; Ohki, Hitoshi; Naito, Hiroyuki
IN
     Daiichi Pharmaceutical Co., Ltd., Japan
PA
SO
     U.S., 51 pp., Cont.-in-part of Appl. No. PCT/JP98/00300.
     CODEN: USXXAM
DT
     Patent
LΑ
    English
FAN.CNT 3
     PATENT NO.
                      KIND
                            DATE
                                           APPLICATION NO.
                                                            DATE
PΙ
                            20010102
                                           US 1999-359419
                                                            19990723
    US 6169086
                       В1
    WO 9832739
                            19980730
                                           WO 1998-JP300
                       A1
                                                            19980126
            AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, GM, GW, HU, ID,
             IL, IS, JP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL,
             RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG,
             KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI,
             FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM,
             GA, GN, ML, MR, NE, SN, TD, TG
                            20030422
                                           US 2000-688787
    US 6552018
                       В1
                                                            20001017
PRAI JP 1997-12116
                            19970127
                       Α
    WO 1998-JP300
                            19980126
                       A2
                            19980724
     JP 1998-208807
                       Α
    US 1999-359419
                            19990723
                       Α3
OS
    MARPAT 134:86238
    Title compds. [I; R = CR3:CR4CHR5GZ; R1, R2 = H, halo, OH, alkoxy, NH2,
AB
     alkylamino, aryl, alkyl; R3,R4 = H, halo, alkoxy, NH2, alkylamino, aryl,
     alkyl; R5 = H, alkyl, alkenyl, alkynyl, aryl(alkyl); Q = C(:NH)NH2,
     cycloalkyl, Ph, or monocyclic heterocycle (excluding pyrimidinyl bonded at
     the 2-position); G = at CHR5-N-attached azacycloalkylidene or
     -N-Z-attached diazacycloalkylidene; Z = Ph, heterocyclyl, etc.] were
    prepd. Thus, 2-amino-4,6-dichloropyrimidine was aminated by H2NH2 and the
    product cyclocondensed with MeCOC(:CHOEt)CO2Et to give I (Q = Z1R6, R1 =
    H, R2 = Me, Z1 = 2-aminopyrimidine-4,6-diyl)(II; R = CO2Et, R6 = Cl) which
    was converted in 5 steps to II [R = (E)-CH:CHCHO, R6 = NMe2]. The latter
    was reductively aminated by 1-(3,5-difluorophenyl)piperazine to give title
     compd. III. Data for biol. activity of I were given.
IT
    210992-71-5P 210992-84-0P 256930-33-3P
     316359-45-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. of pyrazole derivs. as antitumor agents)
RN
     210992-71-5 CAPLUS
CN
     1H-Pyrazole-4-carboxylic acid, 1-[2-[[(4-methoxyphenyl)methyl]amino]-4-
```

pyrimidinyl]-5-methyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 210992-84-0 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-[2-amino-6-(phenylmethoxy)-4-pyrimidinyl]-5-methyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 256930-33-3 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-(2-amino-6-chloro-4-pyrimidinyl)-5-methyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 316359-45-2 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-[2-amino-6-[[(4-methoxyphenyl)methyl]amino]-4-pyrimidinyl]-5-methyl-, ethyl ester (9CI) (CA INDEX NAME)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L4
     ANSWER 11 OF 20 CAPLUS COPYRIGHT 2003 ACS
ΑN
     2000:824247 CAPLUS
DN
     133:350246
     Phenylpyridinylimidazoles and (phenylimidazolyl)pyrimidines having
ΤI
     cytokine inhibitory activity
IN
     Liverton, Nigel J.; Claremon, David A.; Theberge, Cory R.
    Merck & Co., Inc., USA
PΑ
SO
     PCT Int. Appl., 53 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                      KIND
                           DATE
                                           APPLICATION NO.
                                                            DATE
                            20001123
PΙ
    WO 2000069848
                                           WO 2000-US12973 20000511
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             ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV,
             MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG,
             SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW,
            AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
    US 6492516
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                                           US 2000-564272
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                                      EP 2000-932319
                                                            20000511
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PRAI US 1999-134164P
                            19990514
                       Ρ
    WO 2000-US12973
                            20000511
                       W
    MARPAT 133:350246
OS
    Title compds. I (Y = OH, alkoxy, substituted amino, etc.; R3 = H,
AB
    aralkylamino, alkylamino, etc.; R4, R5, R6 = H, halo, OH, CF3, NH2, etc.;
    Q = CH, N) were prepd. Thus, I [Y = EtO, R3 = (S)-(.alpha.-
    methylbenzyl)amino, R4 = R5 = H, R6 = CF3, Q = N] was prepd. in 4 steps
    starting from 3-(trifluoromethyl)benzamidoxime and Et propiolate.
     306297-38-1P 306297-40-5P 306297-43-8P
    306297-45-0P 306297-48-3P
    RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use);
    BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent);
    USES (Uses)
        ((phenylimidazolyl)pyrimidines having cytokine inhibitory activity)
RN
    306297-38-1 CAPLUS
CN
    1H-Imidazole-4-carboxylic acid, 1-[2-[[(1S)-1-phenylethyl]amino]-4-
    pyrimidinyl]-2-[3-(trifluoromethyl)phenyl]-, ethyl ester (9CI) (CA INDEX
    NAME)
```

RN 306297-40-5 CAPLUS

CN 1H-Imidazole-4-carboxylic acid, 1-[2-[[(1S)-1-phenylethyl]amino]-4-pyrimidinyl]-2-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 306297-43-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[1-[2-[[(1S)-1-phenylethyl]amino]-4-pyrimidinyl]-2-[3-(trifluoromethyl)phenyl]-1H-imidazol-4-yl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 306297-45-0 CAPLUS

CN 1H-Imidazole-4-carboxylic acid, 2-phenyl-1-[2-[[(1S)-1-phenylethyl]amino]-4-pyrimidinyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 306297-48-3 CAPLUS

CN 1H-Imidazole-4-carboxylic acid, 2-phenyl-1-[2-[[(1S)-1-phenylethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

INDEX NAME)

RN 306297-59-6 CAPLUS

CN 1H-Imidazole-4-carboxamide, N-[2-(dimethylamino)ethyl]-1-[2-[[(1S)-1-phenylethyl]amino]-4-pyrimidinyl]-2-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 306297-62-1 CAPLUS

CN 1H-Imidazole-4-carboxamide, N-(3R)-1-azabicyclo[2.2.2]oct-3-yl-1-[2-[[(1S)-1-phenylethyl]amino]-4-pyrimidinyl]-2-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 306297-68-7 CAPLUS

CN lH-Imidazole-4-carboxylic acid, 1-[2-[(1,1-dimethylethyl)amino]-4-pyrimidinyl]-2-[3-(trifluoromethyl)phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 306297-71-2 CAPLUS

CN lH-Imidazole-4-carboxylic acid, l-[2-(cyclobutylamino)-4-pyrimidinyl]-2-[3-(trifluoromethyl)phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 306297-74-5 CAPLUS

CN 1H-Imidazole-4-carboxylic acid, 1-[2-[[2-(2-chlorophenyl)ethyl]amino]-4-pyrimidinyl]-2-[3-(trifluoromethyl)phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Eto-C
$$N$$
 CF_3 CI_N $NH-CH_2-CH_2$

RN 306297-77-8 CAPLUS

CN 1H-Imidazole-4-carboxylic acid, 1-[2-[[(2-fluorophenyl)methyl]amino]-4-pyrimidinyl]-2-[3-(trifluoromethyl)phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 306297-82-5 CAPLUS

CN 1H-Imidazole-4-carboxamide, N-[2-(dimethylamino)ethyl]-2-phenyl-1-[2-[((1S)-1-phenylethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L4
     ANSWER 12 OF 20 CAPLUS COPYRIGHT 2003 ACS
AN
     2000:157715 CAPLUS
     132:194285
DN
ΤI
     Preparation of [(sulfonamidooxopyrrolidino)methyl]benzamidines as factor
     Xa inhibitors
IN
     Ewing, William R.; Becker, Michael R.; Choi-Sledeski, Yong Mi; Pauls,
     Heinz W.; McGarry, Daniel G.; Davis, Roderick S.; Spada, Alfred P.
PA
     Rhone-Poulenc Rorer Pharmaceuticals, Inc., USA
SO
     U.S., 47 pp., Cont.-in-part of U.S. 5,731,315.
     CODEN: USXXAM
DT
     Patent
LA
     English
FAN.CNT 3
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                             DATE
                                            APPLICATION NO.
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     US 6034093
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             LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL; PT, RO, RU, SD, SE,
             SG, SI
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             IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN
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     US 5958918
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     WO 9824784
                             19980611
                                            WO 1997-US22414 19971201
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             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US,
             UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
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                             19960607
     US 1996-761414
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     US 1997-976034
                        A2
     WO 1997-US22414
                       A2
                             19971201
     WO 1996-US1816
                       A1
                             19960607
OS
     MARPAT 132:194285
AΒ
     R4NHZZ1(CH2)nZ2NRSO2R1 [I; R,R4 = H, (un)substituted alkyl,
     -(hetero)arylalkyl, etc.; R1 = (un)substituted thienyl or -Ph; Z = CH2 or
     C(:NR5); R5 = R1 = (un) substituted thienyl or -Ph; z1 = (un) substituted
     phenylene or -heteroarylene; Z2 = (un)substituted 1,3-cyclobutylene,
     -pyrrolidinediyl, -piperidinediyl, etc.; n = 0-3] were prepd. Thus,
     (S)-H2NCH2CH2CH(NHCO2CMe3)CO2H was lactamized and the product N-alkylated
     by 3-(NC)C6H4CH2Br to give, after deprotection, (S)-3-(3-amino-2-oxo-1-
     pyrrolidinyl)benzonitrile which was amidated by benzo[b]thiophene-2-
     sulfonyl chloride (prepn. given) and the product treated with HCl/EtOH/NH3
     to give title compd. (S)-II. Data for biol. activity of I were given.
ΙT
     205054-21-3P 205054-23-5P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of [(sulfonamidooxopyrrolidino)methyl]benzamidines as factor Xa
        inhibitors)
```

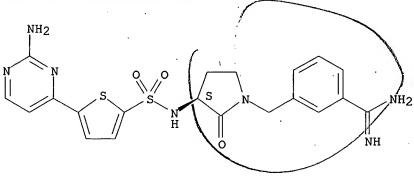
RN 205054-21-3 CAPLUS

CN Benzenecarboximidamide, 3-[[(3S)-3-[[[5-(2-amino-4-pyrimidinyl)-2-thienyl]sulfonyl]amino]-2-oxo-1-pyrrolidinyl]methyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 205054-20-2 CMF C20 H21 N7 O3 S2

Absolute stereochemistry.



CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 205054-23-5 CAPLUS

CN Benzenecarboximidamide, 3-[[(3S)-3-[[[5-(2-amino-4-pyrimidinyl)-2-thienyl]sulfonyl]methylamino]-2-oxo-1-pyrrolidinyl]methyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 205054-22-4 CMF C21 H23 N7 O3 S2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

IT 205055-76-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of [(sulfonamidooxopyrrolidino)methyl]benzamidines as factor Xa
inhibitors)

RN 205055-76-1 CAPLUS

CN 2-Thiophenesulfonamide, 5-(2-amino-4-pyrimidinyl)-N-[(3S)-1-[(3-cyanophenyl)methyl]-2-oxo-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L4
     ANSWER 13 OF 20 CAPLUS COPYRIGHT 2003 ACS
AN
     2000:84798 CAPLUS
DN
     132:137383
     Preparation of pyrazole derivatives as antitumor agents
ΤI
IN
     Ejima, Akio; Ohsuki, Satoru; Ohki, Hitoshi; Naito, Hiroyuki; Makino, Chie
     Daiichi Pharmaceutical Co., Ltd., Japan
PΑ
SO
     PCT Int. Appl., 189 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     Japanese
FAN.CNT 3
     PATENT NO.
                      KIND
                            DATE
                                            APPLICATION NO.
                                                             DATE
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                                           WO 1999-JP3962
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             MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM,
             TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD,
             RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK,
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     US 6573377
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PRAI JP 1998-208807
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                       Α
     JP 1998-274459
                       Α
                            19980929
     WO 1999-JP3962
                       W
                            19990723
OS
     MARPAT 132:137383
     The title compds. I [R1 = H, halo, etc.; R2 = H, halo, OH, etc.; R3 = H,
AΒ
     amino, alkoxy, etc.; R4 = H, halo, alkylamino, etc.; R5 = H, alkyl, etc.;
     Q = heterocyclic ring, etc.; G = heterocyclic ring (further details on
     said ring are given)] are prepd. Compds. of this invention in vitro
     showed IC50 values of 0.6 ng/mL to 35 ng/mL against the growth of lung
     tumor cells.
IT
     256930-33-3P 256930-74-2P 256931-29-0P
     256931-34-7P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. of pyrazole derivs. as antitumor agents)
RN
     256930-33-3 CAPLUS
     1H-Pyrazole-4-carboxylic acid, 1-(2-amino-6-chloro-4-pyrimidinyl)-5-methyl-
CN
```

, ethyl ester (9CI) (CA INDEX NAME).

RN 256930-74-2 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-(2-amino-6-chloro-5-methoxy-4-pyrimidinyl)-5-methyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 256931-29-0 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-[6-chloro-2-[[(4-methoxyphenyl)methyl]amino]-4-pyrimidinyl]-5-ethyl-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ N & & & \\ & & & \\ N & & \\ NH-CH_2 & & \\ & & \\ MeO-C & & Et \\ & & \\ O & & \\ \end{array}$$

RN 256931-34-7 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-(2-amino-6-chloro-4-pyrimidinyl)-5-ethyl-, methyl ester (9CI) (CA INDEX NAME)

```
L4
    ANSWER 14 OF 20 CAPLUS COPYRIGHT 2003 ACS
AN
     1998:527319 CAPLUS
     129:161560
DN
TI
     Preparation of pyrazole derivatives as antitumor agents
     Ejima, Akio; Ohsuki, Satoru
IN
     Daiichi Pharmaceutical Co., Ltd., Japan
PA
SO
     PCT Int. Appl., 90 pp.
     CODEN: PIXXD2
DT
     Patent
LА
    Japanese
FAN.CNT 3
     PATENT NO.
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                                                             DATE
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             KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI,
             FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM,
             GA, GN, ML, MR, NE, SN, TD, TG
    AU 9855771
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                            20020511
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    CN 1105707
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PRAI JP 1997-12116
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    WO 1998-JP300
                       W
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    JP 1998-208807
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    US 1999-359419
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                            19990723
OS
    MARPAT 129:161560
    The title compds. [I; R1 and R2 each is hydrogen, halo, hydroxy, alkoxy,
    amino, alkylamino, aryl, or alkyl; R3 and R4 each is hydrogen, halo,
    alkoxy, amino, alkylamino, aryl, or alkyl; R5 is hydrogen, alkyl, alkenyl,
    alkynyl, aryl, or arylalkyl; Q is amidino, cycloalkyl, Ph, or monocyclic
    heterocycle (excluding pyrimidinyl bonded at the 2-position); G is a
    nitrogenous satd. heterocyclyl; Z is Ph, heterocycle, etc.] are prepd.
    are useful as antitumor agents. Thus, compd. (II; W = COCH2) (prepn.
    given) was treated with NaBH4 and refluxed with p-TsOH in THF and treated
    with 1N HCl to give the title compd. II.HCl (W = CH:CH), which showed GI50
    of 10.6 ng/mL when tested with PC-6 tumor cell.
ΙT
    210992-71-5P 210992-84-0P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. of pyrazole derivs. as antitumor agents)
RN
    210992-71-5 CAPLUS
CN
    1H-Pyrazole-4-carboxylic acid, 1-[2-[[(4-methoxyphenyl)methyl]amino]-4-
    pyrimidinyl]-5-methyl-, ethyl ester (9CI) (CA INDEX NAME)
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RN 210992-84-0 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-[2-amino-6-(phenylmethoxy)-4-pyrimidinyl]-5-methyl-, ethyl ester (9CI) (CA INDEX NAME)

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L4
     ANSWER 15 OF 20 CAPLUS COPYRIGHT 2003 ACS
AN
     1998:192127 CAPLUS
DN
     128:243948
     Preparation of heterocyclylsulfonylaminooxopyrrolidinylmethylbenzamidines
ΤI
     and related compounds as Factor Xa inhibitors.
     Ewing, William R.; Becker, Michael R.; Choi-Sledeski, Yong Mi; Pauls,
IN
     Heinz W.; McGarry, Daniel G.; Davis, Roderick S.; Spada, Alfred P.
     Rhone-Poulenc Rorer Pharmaceuticals Inc., USA
PA
SO
     U.S., 36 pp., Cont.-in-part of U.S. 5,612,353.
     CODEN: USXXAM
DT
     Patent
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FAN.CNT 3
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             DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US,
             UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR,
             GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA,
             GN, ML, MR, NE, SN, TD, TG
     AU 9860121
                       A1
                             19980629
                                            AU 1998-60121
                                                              19971201
     AU 727810
                       B2
                             20001221
                                            EP 1997-954779
     EP 894088
                             19990203
                       A1
                                                              19971201
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     CN 1213370
                       Α
                             19990407·
                                            CN 1997-192888
                                                              19971201
     CN 1093856
                       В
                             20021106
     BR 9707489
                       Α
                             19990727
                                            BR 1997-7489
                                                              19971201
     AP 800
                             20000119
                                            AP 1998-1305
                                                              19971201
                       Α
             GH, KE, LS, MW, SD, SZ, UG, ZW
         W:
     JP 2000505815
                       Т2
                             20000516
                                            JP 1998-525861
                                                              19971201
     ZA 9710968
                       ·A
                             19980722
                                            ZA 1997-10968
                                                              19971205
                                            NO 1998-3603
     NO 9803603
                       Α
                             19981005
                                                              19980805
                            20000307
                                            US 1998-130336
     US 6034093
                       Α
                                                              19980806
     CN 1418882
                       A·
                            20030521
                                            CN 2002-103157
                                                              20020201
PRAI US 1995-481024
                       A2
                            19950607
                       A2
     WO 1996-US9816
                             19960607
     US 1996-761414
                       Α.
                             19961206
     US 1997-976034
                       . A2
                             19971121
     WO 1997-US22414
                       W
                             19971201
     MARPAT 128:243948
OS
     Title compds. [I; Arl = Ph, monocyclic heteroaryl; R = H, (substituted)
AΒ
     alkyl, aralkyl, heteroaralkyl, R6O(CH2)x, R6O2C(CH2)x, Y1Y2NCO(CH2)x,
```

AB Title compds. [I; Ar1 = Ph, monocyclic heteroaryl; R = H, (substituted) alkyl, aralkyl, heteroaralkyl, R6O(CH2)x, R6O2C(CH2)x, Y1Y2NCO(CH2)x, Y1Y2N(CH2)x; R1 = H, alkyl, OH, alkoxy, Y1Y2N, halo, CO2R6, CONY1Y2, (CH2)xOR6, (CH2)xNY1Y2, CN; R2, R3 = H, OH, alkoxy, Y1Y2N, halo, CO2R6, CONY1Y2, (CH2)xOR6, (CH2)xNY1Y2, cyano, (substituted) alkyl, cycloalkyl, heterocyclyl, aryl, heteroaryl, etc.; R4 = H, (substituted) alkyl, aralkyl, heteroaralkyl; X1, X11 = H, (substituted) alkyl, aryl, aralkyl,

heteroaryl, heteroaralkyl; X1X11 = 0; X2, X21 = H; X2X21 = 0; X3 = H, OH, (substituted) alkyl, aryl, heteroaryl, aralkyl, heteroaralkyl; X3X1 or X3X11 = atoms to form a 4-7 membered cycloalkyl, heterocyclyl ring; <math>X4 =H, (substituted) alkyl, aralkyl; X5, X51 = H; X5X51 = NR5; R5 = H, R602C, R6O, cyano, R6CO, (substituted) alkyl, NO2, Y1Y2N; Y1, Y2 = H, (substituted) alkyl, aryl, aralkyl, heteroaralkyl; Y1Y2N = 4-7 membered heterocyclyl; X6, X61 = H, R7R8N, R90, R7R8NCO, R7R8NSO2, R7R8NSO2N, R7R8SO2O, R9CO, CO2R6, CONY1Y2, (CH2)xCO2R6, (CH2)xCONY1Y2, (CH2)xOR6, (CH2)xNY1Y2, halo, cyano, NO2; R6 = H, (substituted) alkyl, aralkyl, heteroaralkyl; R7, R8 = H, (substituted) alkyl, etc.; R9 = H, (substituted) alkyl, acyl, etc.; m, n = 0-3; x = 1-5], were prepd. as antithrombotics. Thus, 3-[3-(S)-amino-2-oxopyrrolidin-1ylmethyl]benzonitrile hydrochloride (prepn. given), benzo[b]thiophene-2sulfonyl chloride (prepn. given), and Et3N were stirred in CH2Cl2 to give benzo[b]thiophene-2-sulfonic acid [1-(3-cyanobenzyl)-2-oxopyrrolidin-3-(S)yl]amide. The latter in EtOH/CH2Cl2 was treated with HCl to give a residue which in MeOH was treated with NH3 to give 3-[3-(S)-(benzo[b]thiophene-2-sulfonylamino)-2-oxopyrrolidin-1-ylmethyl]benzamidine trifluoroacetate.

IT 205054-21-3P 205054-23-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of heterocyclylsulfonylaminooxopyrrolidinylmethylbenzamidines and related compds. as Factor Xa inhibitors)

RN 205054-21-3 CAPLUS

CN Benzenecarboximidamide, 3-[[(3S)-3-[[[5-(2-amino-4-pyrimidinyl)-2-thienyl]sulfonyl]amino]-2-oxo-1-pyrrolidinyl]methyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 205054-20-2 CMF C20 H21 N7 O3 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 205054-23-5 CAPLUS

CN Benzenecarboximidamide, 3-[[(3S)-3-[[[5-(2-amino-4-pyrimidinyl)-2-thienyl]sulfonyl]methylamino]-2-oxo-1-pyrrolidinyl]methyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 205054-22-4 CMF C21 H23 N7 O3 S2

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

IT 205055-76-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of heterocyclylsulfonylaminooxopyrrolidinylmethylbenzamidines and related compds. as Factor Xa inhibitors)

RN 205055-76-1 CAPLUS

CN 2-Thiophenesulfonamide, 5-(2-amino-4-pyrimidinyl)-N-[(3S)-1-[(3-cyanophenyl)methyl]-2-oxo-3-pyrrolidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2003 ACS

AN 1993:147494 CAPLUS

DN 118:147494

TI The chemistry of 5-oxodihydroisoxazoles. III. Synthesis of further annelated pyrimidines

AU Prager, Rolf H.; Rosenzweig, Teresa K.; Singh, Yogendra

CS Sch. Phys. Sci., Flinders Univ. South Australia, Adelaide, 5001, Australia

SO Australian Journal of Chemistry (1992), 45(11), 1825-32 CODEN: AJCHAS; ISSN: 0004-9425

DT Journal

LA English

OS CASREACT 118:147494

The synthesis of some 2-heterocyclyl-5-oxo-2,5-dihydroisoxazole-4-carboxylates is reported, where the heterocycle is pyridin-2-yl, triazin-2-yl (I), pyrimidin-4-yl (II), quinolin-2-yl (III) (R1 = H, OMe; R2 = Me, Ph), or phthalazin-1-yl (IV), as is their base-catalyzed rearrangement to the corresponding annelated pyrimidines.

IT 145771-17-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and base-induced rearrangement of)

RN 145771-17-1 CAPLUS

CN 4-Isoxazolecarboxylic acid, 2-(2,6-diamino-4-pyrimidinyl)-2,5-dihydro-5-oxo-, ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2003 ACS

AN 1992:448481 CAPLUS

DN 117:48481

TI Synthesis of some new heterocyclic compounds derived from 2-amino-4-hydrazino-6-substituted pyrimidines

AU Seada, M.; Abdel-Rahman, R. M.; El-Behairy, M.; Hanafy, Fatin

CS Fac. Educat., Ain Shams Univ., Roxy, Egypt

SO Asian Journal of Chemistry (1992), 4(3), 604-14 CODEN: AJCHEW; ISSN: 0970-7077

DT Journal

LA English

AB A no. of new heterocyclic compds. contg. 2-amino-6-substituted pyrimidin-4-yl moiety were prepd. from the reactions of 2-amino-4-hydrazinopyrimidines I (R = Cl, Me). The structures of the prepd. compds. were established by elemental and spectral anal.

IT 93351-00-9P 142077-31-4P 142077-32-5P 142077-33-6P

RN 93351-00-9 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 5-amino-1-(2-amino-6-methyl-4-pyrimidinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 142077-31-4 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-(2-amino-6-chloro-4-pyrimidinyl)-4,5-dihydro-3-methyl-5-oxo-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H_2N & N & N & Me \\ \hline & N & & & \\ & & O & C-OEt \\ \hline & & & O \end{array}$$

RN 142077-32-5 CAPLUS

CN 3-Pyridazinecarboxylic acid, 1-(2-amino-6-chloro-4-pyrimidinyl)-1,4,5,6-tetrahydro-6-oxo- (9CI) (CA INDEX NAME)

RN 142077-33-6 CAPLUS

CN 3-Pyridazinecarboxylic acid, 1-(2-amino-6-methyl-4-pyrimidinyl)-1,4,5,6-tetrahydro-6-oxo- (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2003 ACS

AN 1972:540047 CAPLUS

DN 77:140047

TI Synthetic penicillins

IN Saikawa, Isamu; Hori, Takako; Maeda, Toyoo; Osada, Tamiko; Momoi, Kaishu; Sakamoto, Mayumi; Watanabe, Isao; Fujii, Fumiko; Miyajima, Hitoko

PA Toyama Chemical Industry Co., Ltd.

SO Jpn. Tokkyo Koho, 5 pp.

CODEN: JAXXAD

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI JP 47029918

B4 19720804 JP 1969-104304 19691226

AB The title compds. (I), antibacterials stable against an acid, were prepd. by treating 6-aminopenicillanic acid (II) with 5-substituted 1,2,4-oxadiazole-3-carboxylic acid derivs. E.g., 5-methyl-1,2,4-oxadiazole-3-carbonyl azide in AcOEt was treated with 1.6 g II, NEt3, in CH2Cl2 to give 0.23 g I (R = Me). (R = Ph, 4-OMeC6H4, 2-furyl, 4-pyridyl, 2-amino-5-pyrimidyl) were similarly prepd.

IT 38030-11-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 38030-11-4 CAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[5-(2-amino-5-pyrimidinyl)-1,2,4-oxadiazol-3-yl]carbonyl]amino]-3,3-dimethyl-7-oxo-, [2S-(2.alpha.,5.alpha.,6.beta.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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L4
     ANSWER 19 OF 20 CAPLUS COPYRIGHT 2003 ACS
AN
     1964:440468 CAPLUS
DN
     61:40468
OREF 61:7025f-h,7026a-d
ΤI
     4-(1-Pyrazolyl)pyrimidines
     Shirakawa, Kenzo; Tsujikawa, Teruaki
IN
PA
     Takeda Chemical Industries, Ltd.
SO
     6 pp.
DT
    Patent
LA
    Unavailable
     PATENT NO.
                      KIND DATE
                                           APPLICATION NO.
                                                            DATE
PΙ
     JP 39005040
                            19640420
                                           JP
                                                            19600330
    A mixt. of 2-amino-4-hydrazino-6-methylpyrimidine 1.4, H2O 30, and
AB
     acetylacetone 1.1 parts is boiled 15 min. to give 1.7 parts
     2-amino-4-(3,5-dimethyl-1-pyrazolyl)-6-methylpyrimidine, columns, m.
     114-16.degree. (ligroine). Similarly prepd. are: 2-amino-4-(4-cyanc-5-
     amino-1-pyrazolyl)-6-methylpyrimidine (needles, m. 246-7.degree.);
    2-amino-4-(4-ethoxycarbonyl-5-amino-1-pyrazolyl)-6-methylpyrimidine
     [needles, m. 200-2.degree. (dil. EtOH)]; 2-amino-4-(4-ethoxycarbonyl-5-
    methyl-1-pyrazolyl)-6-methylpyrimidine [plates, m. 153-5.degree. (dil.
     EtOH)]; 2-anilino-4-(3,5-dimethyl-1-pyrazolyl)-6-methylpyrimidine [plates,
    m. 112-13.degree. (ligroine)]; 2-anilino-4-(4-cyano-5-amino-1-pyrazolyl)-6-
    methylpyrimidine [needles, m. 267-9.degree. (ethylene glycol monomethyl
    ether)]; 2-anilino-4-(4-ethoxycarbonyl - 5 - methyl - 1 - pyrazolyl - 6 -
    methylpyrimidine [columns, m. 135-6.5.degree. (80% EtOH)];
     2-benzylamino-4-(3,5-dimethyl-1-pyrazolyl)-6-methylpyrimidine (needles, m.
     142.5-3.5.degree.); 2-benzylamino-4-(4-ethoxycarbonyl-5-methyl-1-
    pyrazolyl)-6-methylpyrimidine [plates, m. 143.5-5.degree.
     (C6H6-ligroine)]; 2-benzylamino-4-(4-ethoxycarbonyl-5-amino-1-pyrazolyl)-6-
    methylpyrimidine [flakes, m. 148-50.degree. (dil. EtOH)];
    2-benzylamino-4-(4-cyano-5-amino-1-pyrazolyl)-6-methylpyrimidine (columns,
    m. 203-5.degree.); 2-methylthio-4-(3,5-dimethyl-1-pyrazolyl)-6-
    methylpyrimidine [needles, m. 103-4.degree. (dioxane-H2O)];
     2-methylthio-4-(4-cyano-5-amino - 1 - pyrazolyl) - 6 - methylpyrimidine
     [needles, m. 239-40.degree. (dioxane-H2O)]; 2,4-bis(3,5-dimethyl-1-
    pyrazolyl)-5,6-trimethylenepyrimidine [needles, m. 113-14.degree.
     (ligroine)]; 2-(3,5-dimethyl-1-pyrazolyl)- 4- (4- ethoxycarbonyl-5-amino-1-
    pyrazolyl)-5,6-trimethylenepyrimidine [columns, m. 182-3.degree. (ethylene
    glycol monomethyl ether)]; 2-(3,5-dimethyl-1-pyrazolyl)-4-(4-cyano-5-
    amino- 1-pyrazolyl)- 5,6-trimethylenepyrimidine [granules, m.
    249-52.degree. (dil. AcOH)]; 2-(3,5-dimethyl-1-pyrazolyl)-4-(4-
     ethoxycarbonyl-5-methyl- 1 - pyrazolyl) - 5,6-trimethylenepyrimidine
     [plates, m. 159.5-61.degree. (C6H6)]; 2,4-bis-(3,5-dimethyl-1-pyrazolyl)-6-
    methylpyrimidine [needles, m. 117-19.degree. (dil. EtOH)];
     2-(3,5-dimethyl-1-pyrazolyl)-4-(4-cyano-5-amino-1-pyrazolyl)-6-
    methylpyrimidine [needles, m. 245-7.degree. (AcOH)]; 2-(3,5-dimethyl-1-
    pyrazolyl)-4-(4-ethoxycarbonyl-5-amino-1-pyrazolyl)-6-methylpyrimidine
     [needles, m. 177-9.degree. (AcOH)]; 2-(3,5-dimethyl-1-pyrazolyl)-4-(4-
     ethoxycarbonyl-5-methyl-1-pyrazolyl)-6-methylpyrimidine [m. 160-1.degree.
          AcOH)]; 2,4-bis(3,5-dimethyl- 1 - pyrazolyl)- 6- phenylpyrimidine
     [needles, m. 153-4.degree. (dil. EtOH)]; 2-(3,5-dimethyl-1-pyrazolyl)-4-
     (4-cyano-5-amino-1-pyrazolyl)-6-phenylpyrimidine [needles, m.
     242-3.degree. (AcOH)]; 2-(3,5-dimethyl-1-pyrazolyl)-4-(4-ethoxycarbonyl-5-
    methyl-1-pyrazolyl)-6-(phenylpyrimidine [needles m. 165-6.degree. (AcOH)];
    2-(3,5-dimethyl-1-pyrazolyl)-4-(4-ethoxycar-bonyl-5-amino-1-pyrazolyl)-6-
    phenylpyrimidine [needles m. 187-8.degree. (AcOH)]; 2-(3,5-dimethyl-1-
    pyrazolyl)-4-(4-ethoxycarbonyl-5-methyl-1-pyrazolyl)-5,6-
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tetramethylenepyrimidine [needles, m. 130-3.degree. (dil. AcOH)]; 2-(3,5-dimethyl-1-pyrazolyl)-4-(4-ethoxycarbonyl - 5- amino- 1 pyrazolyl) - 5,6 - tetramethylpyrimidine [flakes, m. 197-8.degree. (BuOH)]; 2,4-bis(3,5-dimethyl-1-pyrazolyl)-5,6-tetramethylenepyrimidine [m. 130.degree. (dil. AcOH)]; 2-(3,5 - dimethyl - 1 - pyrazolyl) - 5,6 tetramethylenepyrimidine [needles, m. 225.degree. (AcOH)]; 2-anilino-4-(4-ethoxycarbonyl-5-amino-1-pyrazolyl)-6-methylpyrimidine [m. 146-7.degree. (dil. AcOH)]; 2 - hydroxy - 4 - (3,5 - dimethyl - 1 pyrazolyl)pyrimidine [columns, m. 288-9.degree. (dil. EtOH)]; 2-hydroxy-4-(4-cyano-5-amino-1-pyrazolyl)-6-methylpyrimidine [needles, m. >300.degree. (Me Cellosolve)]; 2-hydroxy-4-(4-ethoxycarbonyl-5-amino-1pyrazolyl)-6-methylpyrimidine [needles, m. 298.degree. (Me Cellosolve)]; 2-amino-4-(3-methyl-5-phenyl-1 - pyrazolyl)- 6-methylpyrimidine [needles, m. 189-90.degree. (dil. EtOH)]; 2-amino-4-(4-ethoxycarbonyl-5-phenyl-1pyrazolyl)-6-methylpyrimidine [columns m. 144-5.degree. (dil. EtOH)]. The products are useful as antituberculous, antitumor, and antispasmodic drugs.

IT 91644-40-5, Pyrazole-4-carboxylic acid, 1-(2-amino-6-methyl-4 pyrimidinyl)-5-methyl-, ethyl ester 92555-72-1,
 Pyrazole-4-carboxylic acid, 1-(2-amino-6-methyl-4-pyrimidinyl)-5-phenyl 93351-00-9, Pyrazole-4-carboxylic acid, 5-amino-1-(2-amino-6 methyl-4-pyrimidinyl)-, ethyl ester 93871-87-5,
 Pyrazole-4-carboxylic acid, 1-(2-anilino-6-methyl-4-pyrimidinyl)-5-methyl-, ethyl ester 94069-65-5, Pyrazole-4-carboxylic acid,
 5-amino-1-[2-(benzylamino)-6-methyl-4-pyrimidinyl]-, ethyl ester
 94378-89-9, Pyrazole-4-carboxylic acid, 1-[2-(benzylamino)-6 methyl-4-pyrimidinyl]-5-methyl-, ethyl ester 94711-75-8,
 Pyrazole-4-carboxylic acid, 5-amino-1-(2-anilino-6-methyl-4-pyrimidinyl)-,
 ethyl ester

(prepn. of)

RN 91644-40-5 CAPLUS

CN Pyrazole-4-carboxylic acid, 1-(2-amino-6-methyl-4-pyrimidinyl)-5-methyl-, ethyl ester (7CI) (CA INDEX NAME)

RN 92555-72-1 CAPLUS

CN Pyrazole-4-carboxylic acid, 1-(2-amino-6-methyl-4-pyrimidinyl)-5-phenyl-(7CI) (CA INDEX NAME)

RN 93351-00-9 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 5-amino-1-(2-amino-6-methyl-4-pyrimidinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 93871-87-5 CAPLUS

CN Pyrazole-4-carboxylic acid, 1-(2-anilino-6-methyl-4-pyrimidinyl)-5-methyl-, ethyl ester (7CI) (CA INDEX NAME)

RN 94069-65-5 CAPLUS

CN Pyrazole-4-carboxylic acid, 5-amino-1-[2-(benzylamino)-6-methyl-4-pyrimidinyl]-, ethyl ester (7CI) (CA INDEX NAME)

RN 94378-89-9 CAPLUS

CN Pyrazole-4-carboxylic acid, 1-[2-(benzylamino)-6-methyl-4-pyrimidinyl]-5-methyl-, ethyl ester (7CI) (CA INDEX NAME)

RN 94711-75-8 CAPLUS

CN Pyrazole-4-carboxylic acid, 5-amino-1-(2-anilino-6-methyl-4-pyrimidinyl)-, ethyl ester (7CI) (CA INDEX NAME)

- L4ANSWER 20 OF 20 CAPLUS COPYRIGHT 2003 ACS
- AN 1964:68217 CAPLUS
- DN 60:68217
- OREF 60:12009h,12010a-h,12011a-c
- ΤI Pyrimidine derivatives. XII. 2-(1-Pyrazolyl)pyrimidines. 2
- ΑU Shirakawa, Kenzo; Tsujikawa, Teruaki
- CS Takeda Res. Lab., Osaka, Japan
- SO Takeda Kenkyusho Nenpo (1963), 22, 27-46 CODEN: TDKNAF; ISSN: 0371-5973
- DT Journal
- LА
- Unavailable AB Boiling of a mixt. of 8 g. 2-(4-ethoxycarbonyl-5-methyl-1-pyrazolyl)-4hydroxy-6-phenylpyrimidine, 70 cc. 4% NaOH, and 70 cc. EtOH for 30 min. gives 60.3% 2-(4-carboxy-5-methyl-1-pyrazolyl)-4-hydroxy-6phenylpyrimidine, m. 320.degree. (decompn.) (AcOH). Similarly prepd. are 2-(4-carboxy-5-amino-1-pyrazolyl)-4-hydroxy-6-methylpyrimidine [m. 229.degree. (decompn.) (dil. AcOH)], 2-(4-carboxy-5-amino-1-pyrazolyl)-4hydroxy-5,6-tetramethylenepyrimidine [m. 250.degree. (decompn.) (EtOCH2CH2OH)], and 2-(3,5-dimethyl-1-pyrazolyl)-4-hydroxy-5carboxypyrimidine [m. 255.degree. (decompn.) (MeOCH2CH2OH)] in 64%, 17%, and 34.4% yields, resp. They are dissolved in CHCl3 and treated with Cl or Br to give corresponding chlorinated or brominated products: (product, m.p., and % yield given): 2-(3,5-dimethyl-4-chloro-1-pyrazolyl)-4-hydroxy-5-chloro-6-methylpyrimidine, 248-51.degree. (EtOH), 52.2; 2-(3,5-dimethyl-4-bromo-1-pyrazolyl)-4-hydroxy-5-bromo-6-methylpyrimidine, 246-8.degree. (dil. AcOH), 83; 2-(3,5-dimethyl-4-bromo-1-pyrazolyl)-4-hydroxy-5-bromo-6-phenylpyrimidine, 150-1.degree. (CHCl3), 83; 2-(3-methyl-4-bromo-5-phenyl-1-pyrazolyl)-4-hydroxy-5-bromo-6phenylpyrimidine, 229-31.degree. (PhMe), 67.3; 2-(4-ethoxycarbonyl-5methyl-1-pyrazolyl)-4-hydroxy-5-bromo-6-phenylpyrimidine, 167-9.degree. (dil. EtOH), 85.8%. 4-Hydroxy compds. are treated with POCl3 to give 4-Cl compds. Thus, the following I are prepd. (R, R1, m.p., and % yield given): H, Me, 57.degree. (dil. EtOH), 55; (RR1=) (CH2)3, 131-3.degree. (C6H6-ligroine), 95.5; (RR1=) (CH2)4, 130-2.degree. (ligroine), 58; H, Ph, 117-18.degree. (dil. EtOH), 89. Reaction of I with NH2NH2.H2O gives II (R, R1, m.p., and % yield given): H, Me, 183-4.degree. (BuOH), 72.5; (RR1=) (CH2)3, 1857.degree. (dil. EtOH), 83.5; (RR1=) (CH2)4, 128-32.degree. (dil. EtOH), 81.2; H, Ph, 206-7.degree. (BuOH), 66. synthesis of the following III is also reported (R, R1, R2, R3, R4, appearance, and m.p. given): Me, H, Me, NH2, Me, prisms, 114-16.degree. (ligroine); Me, H, Me, NHPh, Me, plates, 112-13.degree. (ligroine); Me, H, Me, NHCH2Ph, Me, needles, 142.5-3.5.degree. (dil. EtOH); Me, H, Me, SMe, Me, needles, 103-4.degree. (dil. dioxane); Me, H, Me, Me, NH2, needles, 120-3.degree. (MeOCH2CH2OH); Me, H, Me, OH, Me, prisms, 288-9.degree. (decompn.) (EtOH); H, CO2Et, Me, NH2, Me, plates, 153-5.degree. (dil. EtOH); H, CO2Et, Me, NHPh, Me, prisms, 135-6.5.degree. (80% EtOH); H, CO2Et, Me, NHCH2Ph, Me, plates, 143.5-5.degree. (C6H6-ligroine); H, CO2Et, Ph, NH2, Me, prisms, 144-5.degree. (dil. EtOH); H, CO2Et, NH2, NH2, Me, needles, 200-2.degree. (70% EtOH); H, CO2Et, NH2, NHPh, Me, needles, 146-7.degree. (dil. AcOH); H, CO2Et, NH2, NHCH2Ph, Me, leaflets, 148-50.degree. (50% EtOH); H, CO2Et, NH2, OH, Me, needles, 298.degree. (decompn.) (MeOCH2CH2OH); H, CN, NH2, NH2, Me, needles, 251-2.degree. (80% EtOH); H, CN, NH2, NHPh, Me, needles, 2679.degree. (EtOCH2CH2OH); H, CN, NH2, NHCH2Ph, Me, prisms, 203-5.degree. (60% AcOH); H, CN, NH2, SMe, Me, needles, 239-40.degree. (dil. dioxane); H, CN, NH2, OH, Me, needles, >300.degree. (MeOCH2CH2OH). IV are also prepd. (same data): Me, H, Me, H, Me, needles, 117-19.degree. (80% EtOH); Me, H, Me, (R3R4=) (CH2)3, needles, 113-14.degree. (ligroine); Me, H, Me, (R3R4=)(CH2)4, powder,

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103.degree. (dil. AcOH); Me, H, Me, H, Ph, needles, 153-4.degree. (80%
EtOH); H, CO2Et, Me, H, Me, prisms, 160-1.degree. (dil. AcOH); H, CO2Et,
Me, (R3R4=) (CH2)3, plates, 159.5-61.degree. (C6H6); H, CO2Et, Me, (R3R4=)
(CH2)4, needles, 130-3.degree. (dil. AcOH); H, CO2Et, Me, H, Ph, needles,
165-6.degree. (AcOH); H, CO2Et, NH2, H, Me, needles, 177-9.degree. (AcOH);
H, CO2Et, NH2, (R3R4=) (CH2)3, prisms, 182-3.degree. (EtOCH2CH2OH); H,
CO2Et, NH2, (R3R4=) (CH2)4, leaflets, 197-8.degree. (BuOH); H, CO2Et, NH2,
H, Ph, needles, 187-8.degree. (AcOH); H, CN, NH2, H, Me, needles,
245-7.degree. (AcOH); H, CN, NH2, (R3R4=) (CH2)3, powder, 249-50.degree. (dil. AcOH); H, CN, NH2, (R3R4=) (CH2)4, needles, 225.degree. (AcOH); H, CN, NH2, H, Ph, needles, 242-3.degree. (AcOH). The following V are prepd.
(R, R1, R2, R3, and m.p. given): 2-pyridyl, H, CO2Et, NH2, 93-5.degree.
(ligroine); 2-pyridyl, H, CN, NH2, 186-9.degree. (EtCH2CH2OH); a, Me, H,
Me, 165-7.degree. (MeOCH2CH2OH); a, H, CO2Et, Me, 160-2.degree.
(MeOCH2CH2OH); a, H, CO2Et, NH2, >300.degree. (MeOCH2CH2OH); a, H, CN,
NH2, >300.degree. (MeOCH2CH2OH); b, H, CO2Et, NH2, 216.degree. (decompn.)
(MeOCH2CH2OH); c, Me, H, Me, 104-5.degree. (MeOCH2CH2OH); c, H, CO2Et,
NH2, 132-5.degree. (MeOCH2CH2OH); d, Me, H, Me, 106-9.degree.
(MeOCH2CH2OH); e, Me, H, Me, 123-4.degree. (EtOH); f, Me, H, Me,
132-3.degree. (EtOH); g, Me, H, Me, 143-5.degree. (dil. EtOH); h, H,
CO2Et, NH2, 130-1.degree. (MeOH); i, H, CO2Et, NH2, 88.degree. (EtOH); j,
Me, H, Me, 237.degree. (dil. EtOH); k, Me, H, Me, 68-70(EtOH); l, Me, H,
Me, -(oil, b4 204.degree.); m. H, CO2Et, NH2, 278.degree. (decompn.)
(MeOCH2CH2OH); o-MeOC6H4, Me, H, Me, -(oil. b14 161-4.degree.):
p-H2NO2SC6H4, Me, H. Me, 228-30.degree. (MeOCH2CH2OH); m-H03SC6H4, Me, H,
Me, 313.degree. (decompn.) (dil. EtOH); p-HO2CCH2C6H4, Me, H, Me,
151-2.5.degree. (dil. EtOH); p-HO2CCH2C6H4, Me, H, Ph, 189-90.degree.
(dil. EtOH). The following VI are prepd. (R and m.p. given): n,
154-6.degree. (EtOH); o, 95-7.degree. (EtOH); p, 240.degree. (decompn.)
(MeSOMe); q, 244.degree. (MeSOMe); a, 272.degree. (MeSOMe); r, 220.degree.
(EtOH). 2-(1-Pyrazolyl)-4-hydroxypyrimidines were effective in inhibiting
growth of Mycobacterium tuberculosis.
91644-40-5, Pyrazole-4-carboxylic acid, 1-(2-amino-6-methyl-4-
pyrimidinyl)-5-methyl-, ethyl ester 92555-72-1,
Pyrazole-4-carboxylic acid, 1-(2-amino-6-methyl-4-pyrimidinyl)-5-phenyl-
93351-00-9, Pyrazole-4-carboxylic acid, 5-amino-1-(2-amino-6-
methyl-4-pyrimidinyl)-, ethyl ester 93435-99-5,
Pyrazole-4-carboxylic acid, 1-(2-amino-6-methyl-4-pyrimidinyl)-5-phenyl-,
ethyl ester 93871-87-5, Pyrazole-4-carboxylic acid,
1-(2-anilino-6-methyl-4-pyrimidinyl)-5-methyl-, ethyl ester
94069-65-5, Pyrazole-4-carboxylic acid, 5-amino-1-[2-(benzylamino)-
6-methyl-4-pyrimidinyl]-, ethyl ester 94378-89-9,
Pyrazole-4-carboxylic acid, 1-[2-(benzylamino)-6-methyl-4-pyrimidinyl]-5-
methyl-, ethyl ester 94711-75-8, Pyrazole-4-carboxylic acid,
5-amino-1-(2-anilino-6-methyl-4-pyrimidinyl)-, ethyl ester
   (prepn. of)
91644-40-5 CAPLUS
Pyrazole-4-carboxylic acid, 1-(2-amino-6-methyl-4-pyrimidinyl)-5-methyl-,
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IT

RN

CN

ethyl ester (7CI) (CA INDEX NAME)

RN 92555-72-1 CAPLUS

CN Pyrazole-4-carboxylic acid, 1-(2-amino-6-methyl-4-pyrimidinyl)-5-phenyl-(7CI) (CA INDEX NAME)

RN 93351-00-9 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 5-amino-1-(2-amino-6-methyl-4-pyrimidinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 93435-99-5 CAPLUS

CN Pyrazole-4-carboxylic acid, 1-(2-amino-6-methyl-4-pyrimidinyl)-5-phenyl-, ethyl ester (7CI) (CA INDEX NAME)

RN 93871-87-5 CAPLUS

CN Pyrazole-4-carboxylic acid, 1-(2-anilino-6-methyl-4-pyrimidinyl)-5-methyl-, ethyl ester (7CI) (CA INDEX NAME)

RN 94069-65-5 CAPLUS

CN Pyrazole-4-carboxylic acid, 5-amino-1-[2-(benzylamino)-6-methyl-4-pyrimidinyl]-, ethyl ester (7CI) (CA INDEX NAME)

RN 94378-89-9 CAPLUS

CN Pyrazole-4-carboxylic acid, 1-[2-(benzylamino)-6-methyl-4-pyrimidinyl]-5-methyl-, ethyl ester (7CI) (CA INDEX NAME)

RN 94711-75-8 CAPLUS

CN Pyrazole-4-carboxylic acid, 5-amino-1-(2-anilino-6-methyl-4-pyrimidinyl)-, ethyl ester (7CI) (CA INDEX NAME)

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FILE 'REGISTRY' ENTERED AT 19:01:10 ON 01 JUL 2003

L1 STRUCTURE UPLOADED

L2 1 S L1 SSS SAM

L3 237 S L1 SSS FUL

FILE 'CAPLUS' ENTERED AT 19:02:12 ON 01 JUL 2003

L4 20 S L3

FILE 'CAOLD' ENTERED AT 19:03:00 ON 01 JUL 2003

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L5 3 L3

=> d 15 1-3 bib, hitstr

L5 ANSWER 1 OF 3 CAOLD COPYRIGHT 2003 ACS
AN CA61:7026d CAOLD
TI 2,6-bis(ethanolamino)pyrimido[5,4-d]pyrimidines
AU Roch, Josef
DT Patent
TI 2,6-bis(ethanolamino)pyrimido[5,4-d]pyrimidines

AU Thomae, Dr. Karl, G.m.b.H.

DT Patent

PATENT NO. KIND DATE

PI DE 1172685

IT 93435-99-5

RN 93435-99-5 CAOLD

CN Pyrazole-4-carboxylic acid, 1-(2-amino-6-methyl-4-pyrimidinyl)-5-phenyl-, ethyl ester (7CI) (CA INDEX NAME)

$$\begin{array}{c|c} H_2N & N & N \\ \hline N & Ph & C-OEt \\ Me & \parallel & O \end{array}$$

L5 ANSWER 2 OF 3 CAOLD COPYRIGHT 2003 ACS

AN CA61:7025f CAOLD

TI 4-(1-pyrazolyl)pyrimidines .

AU Shirakawa, Kenzo; Tsujikawa, T.

PA Takeda Chemical Industries, Ltd.

DT Patent

PATENT NO. KIND DATE

PI JP 64005040 1964

IT 91644-40-5 93351-00-9 93871-87-5

94069-65-5 94378-89-9 94711-75-8

RN 91644-40-5 CAOLD

CN Pyrazole-4-carboxylic acid, 1-(2-amino-6-methyl-4-pyrimidinyl)-5-methyl-, ethyl ester (7CI) (CA INDEX NAME)

RN 93351-00-9 CAOLD

CN 1H-Pyrazole-4-carboxylic acid, 5-amino-1-(2-amino-6-methyl-4-pyrimidinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 93871-87-5 CAOLD

CN Pyrazole-4-carboxylic acid, 1-(2-anilino-6-methyl-4-pyrimidinyl)-5-methyl, ethyl ester (7CI) (CA INDEX NAME)

RN 94069-65-5 CAOLD

CN Pyrazole-4-carboxylic acid, 5-amino-1-[2-(benzylamino)-6-methyl-4-pyrimidinyl]-, ethyl ester (7CI) (CA INDEX NAME)

RN 94378-89-9 CAOLD

CN Pyrazole-4-carboxylic acid, 1-[2-(benzylamino)-6-methyl-4-pyrimidinyl]-5-methyl-, ethyl ester (7CI) (CA INDEX NAME)

RN 94711-75-8 CAOLD

CN Pyrazole-4-carboxylic acid, 5-amino-1-(2-anilino-6-methyl-4-pyrimidinyl)-, ethyl ester (7CI) (CA INDEX NAME)

L5 ANSWER 3 OF 3 CAOLD COPYRIGHT 2003 ACS

AN CA60:12009b CAOLD

TI pyrimidine derivs. - (XI) 2-(pyrazolyl) - pyrimidines (1), (XII) 2-[1-pyrazolyl)pyrimidines (2)

AU Shirakawa, Kenzo; Tsujikawa, T.

IT 91644-40-5 92555-72-1 93351-00-9 93435-99-5 93871-87-5 94069-65-5 94378-89-9 94711-75-8

RN 91644-40-5 CAOLD

CN Pyrazole-4-carboxylic acid, 1-(2-amino-6-methyl-4-pyrimidinyl)-5-methyl-, ethyl ester (7CI) (CA INDEX NAME)

RN 92555-72-1 CAOLD

CN Pyrazole-4-carboxylic acid, 1-(2-amino-6-methyl-4-pyrimidinyl)-5-phenyl-(7CI) (CA INDEX NAME)

RN 93351-00-9 CAOLD

CN 1H-Pyrazole-4-carboxylic acid, 5-amino-1-(2-amino-6-methyl-4-pyrimidinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 93435-99-5 CAOLD

CN Pyrazole-4-carboxylic acid, 1-(2-amino-6-methyl-4-pyrimidinyl)-5-phenyl-, ethyl ester (7CI) (CA INDEX NAME)

RN 93871-87-5 CAOLD

CN Pyrazole-4-carboxylic acid, 1-(2-anilino-6-methyl-4-pyrimidinyl)-5-methyl-, ethyl ester (7CI) (CA INDEX NAME)

RN 94069-65-5 CAOLD

CN Pyrazole-4-carboxylic acid, 5-amino-1-[2-(benzylamino)-6-methyl-4-pyrimidinyl]-, ethyl ester (7CI) (CA INDEX NAME)

RN 94378-89-9 CAOLD

CN Pyrazole-4-carboxylic acid, 1-[2-(benzylamino)-6-methyl-4-pyrimidinyl]-5-methyl-, ethyl ester (7CI) .(CA INDEX NAME)

RN 94711-75-8 CAOLD

CN Pyrazole-4-carboxylic acid, 5-amino-1-(2-anilino-6-methyl-4-pyrimidinyl)-, ethyl ester (7CI) (CA INDEX NAME)

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FILE 'REGISTRY' ENTERED AT 19:01:10 ON 01 JUL 2003

L1 STRUCTURE UPLOADED

L2 1 S L1 SSS SAM

L3 237 S L1 SSS FUL

FILE 'CAPLUS' ENTERED AT 19:02:12 ON 01 JUL 2003

L4 20 S L3

FILE 'CAOLD' ENTERED AT 19:03:00 ON 01 JUL 2003

L5 3 S L3

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COST IN U.S. DOLLARS SINCE FILE TOTAL

FULL ESTIMATED COST . ENTRY SESSION 8.26 248.16

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE 0.00 -13.02

STN INTERNATIONAL LOGOFF AT 19:03:38 ON 01 JUL 2003